A Roadmap for HEP Software and Computing R&D for the 2020s

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ORIGINAL ARTICLE

A Roadmap for HEP Software and Computing R&D for the 2020s

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Abstract
Particle physics has an ambitious and broad experimental programme for the coming decades. This programme requires large investments in detector hardware, either to build new facilities and experiments, or to upgrade existing ones. Similarly, it requires commensurate investment in the R&D of software to acquire, manage, process, and analyse the shear amounts of data to be recorded. In planning for the HL-LHC in particular, it is critical that all of the collaborating stakeholders agree on the software goals and priorities, and that the efforts complement each other. In this spirit, this white paper describes the R&D activities required to prepare for this software upgrade.

Keywords Particle physics · HL-LHC · Computing & software upgrade · Software performance · Machine learning

Introduction

Particle physics has an ambitious experimental programme for the coming decades. The programme supports the strategic goals of the particle physics community that have been laid out by the European Strategy for Particle Physics [138] and by the Particle Physics Project Prioritization Panel (P5) [106] in the United States [112]. Broadly speaking, the scientific goals are:

- Exploit the discovery of the Higgs boson as a precision tool for investigating Standard Model (SM) and Beyond the Standard Model (BSM) physics.
- Study the decays of *b*- and *c*-hadrons, and tau leptons, in the search for manifestations of BSM physics, and investigate matter–antimatter differences.
- Search for signatures of dark matter.
- Probe neutrino oscillations and masses.
- Study the quark–gluon plasma state of matter in heavy-ion collisions.
- Explore the unknown.

The High-Luminosity Large Hadron Collider (HL-LHC) [64, 114, 145] will be a major upgrade of the current LHC [148] supporting the aim of an in-depth investigation of the properties of the Higgs boson and its couplings to other particles (Fig. 1). The ATLAS [2] and CMS [42] collaborations will continue to make measurements in the Higgs sector, while searching for new physics Beyond the Standard Model (BSM). Should a BSM discovery be made, a full exploration of that physics will be pursued. Such BSM physics may help shed light on the nature of dark matter, which we know makes up the majority of gravitational matter in the universe, but which does not interact via the electromagnetic or strong nuclear forces [94].

The LHCb experiment at the LHC [147] and the Belle II experiment at KEK [135] study various aspects of heavy flavour physics (b- and c-quark, and tau-lepton physics), where quantum influences of very high mass particles manifest themselves in lower energy phenomena. Their primary goal is to look for BSM physics, either by studying CP violation (that is, asymmetries in the behaviour of particles and their corresponding antiparticles) or modifications in rate or angular distributions in rare heavy-flavour decays. Current manifestations of such asymmetries do not explain why our universe is so matter dominated. These flavour physics programmes are related to BSM searches through effective field theory, and powerful constraints on new physics keep coming from such studies.

The study of neutrinos, their mass and oscillations, can also shed light on matter–antimatter asymmetry. The DUNE experiment will provide a huge improvement in our

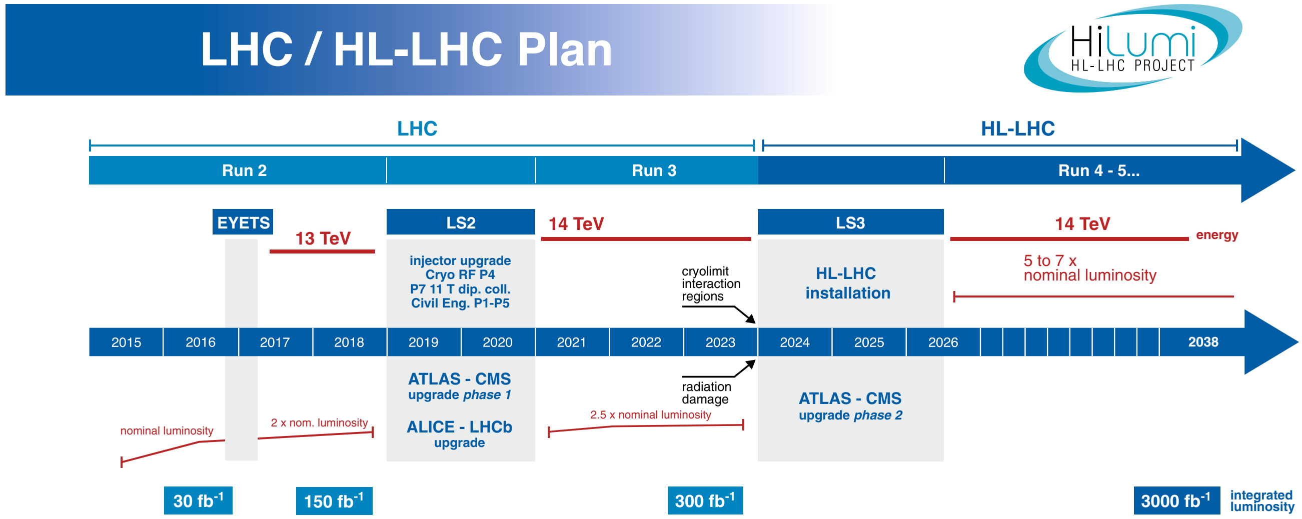


Fig. 1 The current schedule for the LHC and HL-LHC upgrade and run [145]. Currently, the start of the HL-LHC run is foreseen for mid 2026. The long shutdowns, LS2 and LS3, will be used to upgrade both the accelerator and the detector hardware

ability to probe neutrino physics, detecting neutrinos from the Long Baseline Neutrino Facility at Fermilab, as well as linking to astro-particle physics programmes, in particular through the potential detection of supernovas and relic neutrinos. An overview of the experimental programme scheduled at the Fermilab facility is given in Fig. 2.

In the study of the early universe immediately after the Big Bang, it is critical to understand the phase transition between the highly compressed quark–gluon plasma and the nuclear matter in the universe today. The ALICE experiment at the LHC [1] and the CBM [31] and PANDA [105] experiments at the Facility for Antiproton and Ion Research (FAIR) are specifically designed to probe this aspect of nuclear and

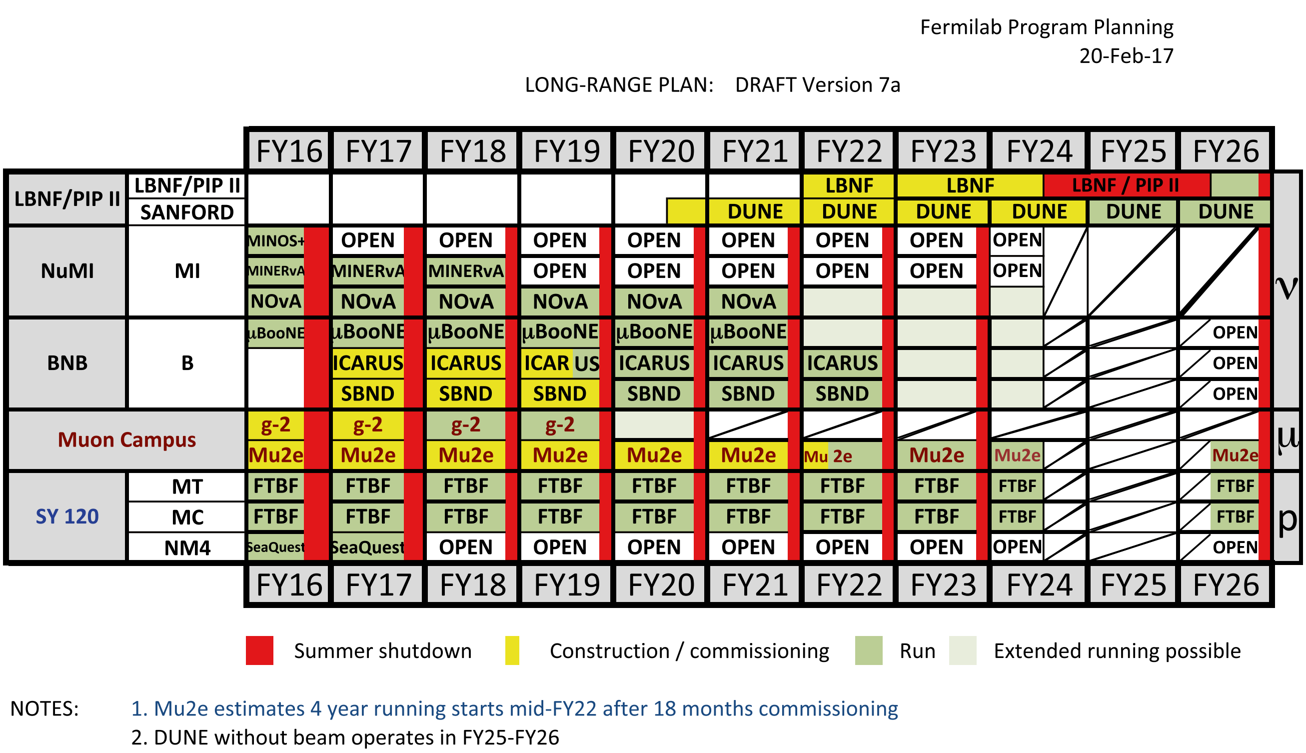


Fig. 2 Run schedule for the Fermilab facility until 2026 [61]

particle physics. In addition ATLAS, CMS and LHCb all contribute to the LHC heavy-ion programme.

These experimental programmes require large investments in detector hardware, either to build new facilities and experiments (e.g., FAIR and DUNE) or to upgrade existing ones (HL-LHC, Belle II). Similarly, they require commensurate investment in the research and development necessary to deploy software to acquire, manage, process, and analyse the data recorded.

For the HL-LHC, which is scheduled to begin taking data in 2026 (Fig. 1) and to run into the 2030s, some 30 times more data than the LHC has currently produced will be collected by ATLAS and CMS. As the total amount of LHC data already collected is close to an exabyte, it is clear that the problems to be solved require approaches beyond simply scaling current solutions, assuming Moore's Law and more or less constant operational budgets. The nature of computing hardware (processors, storage, networks) is evolving with radically new paradigms, the quantity of data to be processed is increasing dramatically, its complexity is increasing, and more sophisticated analyses will be required to maximise physics yield. Developing and deploying sustainable software for future and upgraded experiments, given these constraints, is both a technical and a social challenge, as detailed in this paper. An important message of this report is that a "software upgrade" is needed to run in parallel with the hardware upgrades planned for the HL-LHC in order to take full advantage of these hardware upgrades and to complete the HL-LHC physics programme.

In planning for the HL-LHC in particular, it is critical that all of the collaborating stakeholders agree on the software goals and priorities, and that the efforts complement each other. In this spirit, the HEP Software Foundation (HSF) began a planning exercise in late 2016 to prepare a Community White Paper (CWP) [146] at the behest of the Worldwide LHC Computing Grid (WLCG) project [36]. The role of the HSF is to facilitate coordination and common efforts in HEP software and computing internationally and to provide a structure for the community to set goals and priorities for future work. The objective of the CWP is to provide a roadmap for software R&D in preparation for the HL-LHC and for other HEP experiments on a similar timescale, which would identify and prioritise the software research and development investments required:

- to achieve improvements in software efficiency, scalability and performance, and to make use of advances in CPU, storage and network technologies to cope with the challenges ahead;
- to enable new approaches to computing and software that can radically extend the physics reach of the detectors;
- to ensure the long-term sustainability of the software through the lifetime of the HL-LHC;
- to ensure data and knowledge preservation beyond the lifetime of individual experiments;
- to attract the required new expertise by offering appropriate career recognition to physicists specialising in software development and by an effective training effort to target all software contributors in the community.

The CWP process, organised by the HSF with the participation of the LHC experiments and the wider HEP software and computing community, began with a kick-off workshop at the San Diego Supercomputer Centre (SDSC), USA, in January 2017 and concluded after a final workshop in June 2017 at the Laboratoire d'Annecy de Physique des Particules (LAPP), France, with a large number of intermediate topical workshops and meetings (Appendix A). The entire CWP process involved an estimated 250 participants.

To reach more widely than the LHC experiments, specific contact was made with individuals with software and computing responsibilities in the Fermilab muon and neutrino experiments, Belle II, the Linear Collider community, as well as various national computing organisations. The CWP process was able to build on all the links established since the inception of the HSF in 2014.

Working groups were established on various topics which were expected to be important parts of the HL-LHC roadmap: Careers, Staffing and Training; Conditions Database; Data Organisation, Management and Access; Data Analysis and Interpretation; Data and Software Preservation; Detector Simulation; Data-Flow Processing Frameworks; Facilities and Distributed Computing; Machine Learning; Physics Generators; Security; Software Development, Deployment and Validation/Verification; Software Trigger and Event Reconstruction; and Visualisation. The work of each working group is summarised in this document.

This document is the result of the CWP process. Investing in the roadmap outlined here will be fruitful for the whole of the HEP programme and may also benefit other projects with similar technical challenges, particularly in astrophysics, e.g., the Square Kilometre Array (SKA) [128], the Cherenkov Telescope Array (CTA) [136] and the Large Synoptic Survey Telescope (LSST) [149].

Software and Computing Challenges

Run 2 for the LHC started in 2015 and delivered a proton–proton collision energy of 13 TeV. By the end of LHC Run 2 in 2018, it is expected that about 150 fb^{-1} of physics data will have been collected by both ATLAS and CMS. Together with ALICE and LHCb, the total size of LHC data storage pledged by sites for the year 2017 is around 1 exabyte, as shown in Table 1 from the LHC's Computing

Table 1 Resources pledged by WLCG sites to the 4 LHC experiments for the year 2017 as described at the September 2017 session of the Computing Resources Scrutiny Group (CRSG)

Experiment	2017 disk pledges (PB)	2017 tape pledges (PB)	Total disk and tape pledges (PB)	2017 CPU pledges (kHS06)
ALICE	67	68	138	807
ATLAS	172	251	423	2194
CMS	123	204	327	1729
LHCb	35	67	102	413
Total	400	591	990	5143

Resource Scrutiny Group (CRSG) [91]. The CPU allocation from the CRSG for 2017 to each experiment is also shown.

Using an approximate conversion from HS06 [76] to CPU cores of 10 means that LHC computing in 2017 is supported by about 500k CPU cores. These resources are deployed ubiquitously, from close to the experiments themselves at CERN to a worldwide distributed computing infrastructure, the WLCG [162]. Each experiment has developed its own workflow management and data management software to manage its share of WLCG resources.

To process the data, the 4 largest LHC experiments have written tens of millions of lines of program code over the last 15 years [56, 101, 102, 131]. This has involved contributions from thousands of physicists and many computing professionals, encompassing a wide range of skills and abilities. The majority of this code was written for a single architecture (x86_64) and with a serial processing model in mind. There is considerable anxiety in the experiments that much of this software is not sustainable, with the original authors no longer in the field and much of the code itself in a poorly maintained state, ill-documented, and lacking tests. This code, which is largely experiment-specific, manages the entire experiment data flow, including data acquisition, high-level triggering, calibration and alignment, simulation, reconstruction (of both real and simulated data), visualisation, and final data analysis.

HEP experiments are typically served with a large set of integrated and configured common software components, which have been developed either in-house or externally. Well-known examples include ROOT [29], which is a data analysis toolkit that also plays a critical role in the implementation of experiments' data storage systems, and Geant4 [8], a simulation framework through which most detector simulation is achieved. Other packages provide tools for supporting the development process; they include compilers and scripting languages, as well as tools for integrating, building, testing, and generating documentation. Physics simulation is supported by a wide range of event generators provided by the theory community (PYTHIA [109], SHERPA [69], ALPGEN [95], MADGRAPH [150], HERWIG [144], amongst many others). There is also code developed to support the computing infrastructure itself, such as the CVMFS distributed caching filesystem [28], the Frontier database caching mechanism [63], the XRootD file access software [163] and a number of storage systems (dCache, DPM, EOS). This list of packages is by no means exhaustive, but illustrates the range of software employed and its critical role in almost every aspect of the programme.

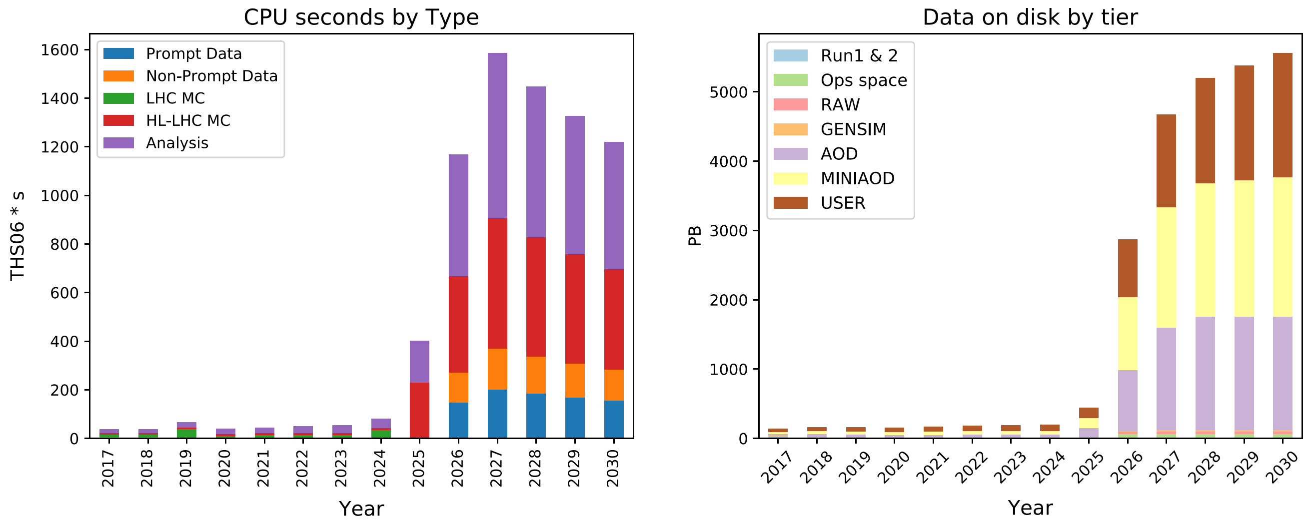
Already in Run 3 LHCb will process more than 40 times the number of collisions that it does today, and ALICE will read out Pb–Pb collisions continuously at 50 kHz. The upgrade to the HL-LHC for Run 4 then produces a step change for ATLAS and CMS. The beam intensity will rise substantially, giving bunch crossings where the number of discrete proton–proton interactions (pileup) will rise to about 200, from about 60 today. This has important consequences for the operation of the detectors and for the performance of the reconstruction software. The two experiments will upgrade their trigger systems to record 5–10 times as many events as they do today. It is anticipated that HL-LHC will deliver about 300 fb^{-1} of data each year.

The steep rise in resources that are then required to manage this data can be estimated from an extrapolation of the Run 2 computing model and is shown in Figs. 3 and 4.

In general, it can be said that the amount of data that experiments can collect and process in the future will be limited by affordable software and computing, and therefore, the physics reach during HL-LHC will be limited by how efficiently these resources can be used.

The ATLAS numbers, in Fig. 4, are particularly interesting as they estimate the resources that will be available to the experiment if a flat funding profile is maintained, taking into account the expected technology improvements given current trends [43]. As can be seen, the shortfall between needs and bare technology gains is considerable: a factor 4 in CPU and a factor 7 in disk in 2027.

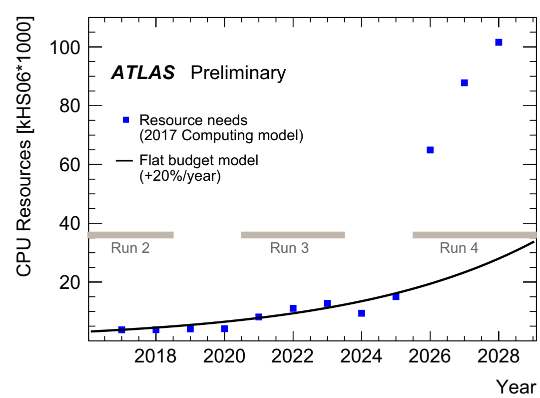
While the density of transistors on silicon continues to increase following Moore's Law (albeit more slowly than in the past), power density constraints have limited the clock speed of processors for more than a decade [47]. This has effectively stalled any progress in the processing capacity of a single CPU core. Instead, increases in potential processing capacity come from increases in the core count of CPUs and wide CPU registers. Alternative processing architectures have become more commonplace. These range from the many-core architecture based on standard x86_64 cores to numerous alternatives such as GPUs. For GPUs, the processing model is very different [46], allowing a much greater fraction of the die to be dedicated to arithmetic calculations, but at a price in programming difficulty and memory handling for the developer that tends to be specific to each processor generation. Further developments may even see the use of FPGAs for more general-purpose tasks. Fully



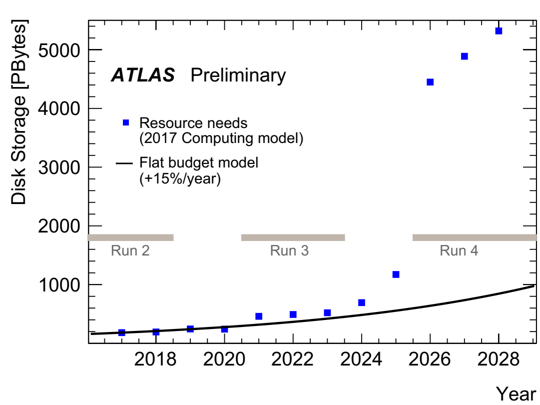
(a) (b)

Fig. 3 CMS estimated CPU (**a**) and disk space (**b**) resources required into the HL-LHC era, using the current computing model with parameters projected out for the next 12 years [120]

Fig. 4 ATLAS resources required into the HL-LHC era, using the current computing model and software performance[14]



(a) Estimated CPU resources (in kHS06) needed for the years 2018 to 2028 for both data and simulation processing. The blue points are estimates based on the current software performance estimates and using the ATLAS computing model parameters from 2017. The solid line shows the amount of resources expected to be available if a flat funding scenario is assumed, which implies an increase of 20% per year, based on the current technology trends.



(b) Estimated total disk resources (in PB) needed for the years 2018 to 2028 for both data and simulation processing. The blue points are estimates based on the current event sizes estimates and using the ATLAS computing model parameters from 2017. The solid line shows the amount of resources expected to be available if a flat funding scenario is assumed, which implies an increase of 15% per year, based on the current technology trends.

exploiting these evolutions requires a shift in programming model to one based on concurrency.

Even with the throttling of clock speed to limit power consumption, power remains a major issue. Low power architectures are in huge demand. At one level this might challenge the dominance of x86_64 by simply replacing it with, for example, AArch64 devices that may achieve lower power costs for the scale of HEP computing needs than Intel has achieved with its Xeon architecture [4, 84, 124]. More extreme is an architecture that would see specialised processing units dedicated to particular tasks, but with possibly large parts of the device switched off most of the time, the so-called dark silicon [80, 97].

Limitations in affordable storage also pose a major challenge, as does the I/O rates of higher capacity hard disks. Network bandwidth will probably continue to increase at the required level, but the ability to use it efficiently will need a closer integration with applications. This will require software developments to support distributed computing (data and workload management, software distribution and data access) and an increasing awareness of the extremely hierarchical view of data, from long latency tape access and medium-latency network access through to the CPU memory hierarchy.

Taking advantage of these new architectures and programming paradigms will be critical for HEP to increase the ability of our code to deliver physics results efficiently, and to meet the processing challenges of the future. Some of this work will be focused on re-optimised implementations of existing algorithms. This will be complicated by the fact that much of our code is written for the much simpler model of serial processing, and without the software engineering needed for sustainability. Proper support for taking advantage of concurrent programming techniques, such as vectorisation and thread-based programming, through frameworks and libraries, will be essential, as the majority of the code will still be written by physicists. Other approaches should examine new algorithms and techniques, including highly parallelised code that can run on GPUs or the use of machine learning techniques to replace computationally expensive pieces of simulation or pattern recognition. The ensemble of computing work that is needed by the experiments must remain sufficiently flexible to take advantage of different architectures that will provide computing to HEP in the future. The use of high-performance computing sites and commercial cloud providers will very likely be a requirement for the community and will bring particular constraints and demand flexibility.

These technical challenges are accompanied by significant human challenges. The software is written by many people in the collaborations, with varying levels of expertise, from a few experts with precious skills to novice coders. This implies organising training in effective coding techniques and providing excellent documentation, examples and support. Although it is inevitable that some developments will remain within the scope of a single experiment, tackling software problems coherently as a community will be critical to achieving success in the future. This will range from sharing knowledge of techniques and best practice to establishing common libraries and projects that will provide generic solutions to the community. Writing code that supports a wider subset of the community than just a single experiment will almost certainly be mandated upon HEP and presents a greater challenge, but the potential benefits are huge. Attracting, and retaining, people with the required skills who can provide leadership is another significant challenge, since it impacts on the need to give adequate recognition to physicists who specialise in software development. This is an important issue that is treated in more detail later in the report.

Particle physics is no longer alone in facing these massive data challenges. Experiments in other fields, from astronomy [130] to genomics [74], will produce huge amounts of data in the future, and will need to overcome the same challenges that we face, i.e., massive data handling and efficient scientific programming. Establishing links with these fields has already started. Additionally, interest from the computing science community in solving these data challenges exists, and mutually beneficial relationships would be possible where there are genuine research problems that are of academic interest to that community and provide practical solutions to ours. The efficient processing of massive data volumes is also a challenge faced by industry, in particular the internet economy, which developed novel and major new technologies under the banner of Big Data that may be applicable to our use cases [12, 116, 121].

Establishing a programme of investment in software for the HEP community, with a view to ensuring effective and sustainable software for the coming decades, will be essential to allow us to reap the physics benefits of the multi-exabyte data to come. It was in recognition of this fact that the HSF itself was set up and already works to promote these common projects and community developments [75].

Programme of Work

In the following, we describe the programme of work being proposed for the range of topics covered by the CWP working groups. We summarise the main specific challenges each topic will face, describe current practices, and propose a number of R&D tasks that should be undertaken to meet the challenges. R&D tasks are grouped in two different timescales: short term (by 2020, in time for the HL-LHC Computing Technical Design Reports of ATLAS and CMS) and longer term actions (by 2022, to be ready for testing or deployment during LHC Run 3).

Physics Generators

Scope and Challenges

Monte-Carlo event generators are a vital part of modern particle physics, providing a key component of the understanding and interpretation of experiment data. Collider experiments have a need for theoretical QCD predictions at very high precision. Already in LHC Run 2, experimental uncertainties for many analyses are at the same level as, or lower than, those from theory. Many analyses have irreducible QCD-induced backgrounds, where statistical extrapolation into the signal region can only come from theory calculations. With future experiment and machine upgrades, as well as reanalysis of current data, measured uncertainties will shrink even further, and this will increase the need to reduce the corresponding errors from theory.

Increasing accuracy will compel the use of higher-order perturbation theory generators with challenging computational demands. Generating Monte Carlo events using Leading Order (LO) generators is only a small part of the overall computing requirements for HEP experiments. Next-to-Leading Order (NLO) event generation, used more during LHC Run 2, is already using significant resources. Higher accuracy theoretical cross sections calculated at Next-to-Next-to-Leading (NNLO), already important in some Run 2 analyses, are not widely used because of computational cost. By HL-LHC the use of NNLO event generation will be more widely required, so these obstacles to their adoption must be overcome. Increasing the order of the generators increases greatly the complexity of the phase space integration required to calculate the appropriate QCD matrix elements. The difficulty of this integration arises from the need to have sufficient coverage in a high-dimensional space (10–15 dimensions, with numerous local maxima); the appearance of negative event weights; and the fact that many terms in the integration cancel, so that a very high degree of accuracy of each term is required. Memory demands for generators have generally been low and initialisation times have been fast, but an increase in order means that memory consumption becomes important and initialisation times can become a significant fraction of the job's run time.

For HEP experiments, in many cases, meaningful predictions can only be obtained by combining higher-order perturbative calculations with parton showers. This procedure is also needed as high-multiplicity final states become more interesting at higher luminosities and event rates. Matching (N)NLO fixed-order calculations to parton shower algorithms can have a very low efficiency, and increases further the computational load needed to generate the necessary number of particle-level events. In addition, many of the current models for the combination of parton-level event generators and parton shower codes are incompatible with requirements for concurrency on modern architectures. It is a major challenge to ensure that this software can run efficiently on next-generation hardware and software systems.

Developments in generator software are mainly done by the HEP theory community. Theorists typically derive career recognition and advancement from making contributions to theory itself, rather than by making improvements to the computational efficiency of generators per se. So, improving the computational efficiency of event generators, and allowing them to run effectively on resources such as High-Performance Computing Facilities (HPCs), will mean engaging with experts in computational optimisation who can work with the theorists who develop generators.

The challenge in the next decade is to advance the theory and practical implementation of event generators to support the needs of future experiments, reaching a new level of theory precision and recognising the demands for computation and computational efficiency that this will bring.

Current Practice

Extensive use of LO generators and parton shower algorithms are still made by most HEP experiments. Each experiment has its own simulation needs, but for the LHC experiments tens of billions of generated events are now used each year for Monte Carlo simulations. During LHC Run 2 more and more NLO generators were used, because of their increased theoretical precision and stability. The raw computational complexity of NLO amplitudes, combined with many-body phase-space evaluations and the inefficiencies of the matching process, leads to a potentially much-increased CPU budget for physics event simulation for ATLAS and CMS.

The use of NLO generators by the experiments today is also limited because of the way the generators are implemented, producing significant numbers of negative event weights. This means that the total number of events the experiments need to generate, simulate, and reconstruct can be many times larger for NLO than for LO samples. At the same time, the experiments budget only a similar number of Monte Carlo simulation events as from the real data. Having large NLO samples is thus not consistent with existing computing budgets until a different scheme is developed that does not depend on negative event weights or produces them only at a significantly reduced rate.

While most event generation is run on "standard" grid resources, effort is ongoing to run more demanding tasks on HPC resources, e.g., W-boson + 5-jet events at the Argonne Mira HPC). However, scaling for efficient running on some of the existing HPC resources is not trivial and requires effort.

Standard HEP libraries such as LHAPDF [88], HepMC [143], and Rivet [152] are used by the generators for integration into the experiments' event generation workflows. These require extensions and sustained maintenance that should be considered a shared responsibility of the theoretical and experimental communities in the context of large-scale experiments. In practice, however, it has been difficult to achieve the level of support that is really needed as there has been a lack of recognition for this work. To help improve the capabilities and performance of generators as used by the experimental HEP programme, and to foster interaction between the communities, the MCnet [57] short-term studentship programme has been very useful. Interested experimental PhD students can join a generator group for several months to work on improving a physics aspect of the simulation that is relevant to their work, or to improve the integration of the generator into an experimental framework.

Research and Development Programme

As the Monte Carlo projects are funded mainly to develop theoretical improvements, and not mainly as "suppliers" to the experimental HEP programme, any strong requests towards efficiency improvements from the experimental community would need to be backed up by plausible avenues of support that can fund contributions from software engineers with the correct technical skills in software optimisation to work within the generator author teams.

In a similar way to the MCnet studentships, a matchmaking scheme could focus on the software engineering side, and transfer some of the expertise available in the experiments and facilities teams to the generator projects. Sustainable improvements are unlikely to be delivered by graduate students "learning on the job" and then leaving after a few months, so meeting the requirement of transferring technical expertise and effort will likely require placements for experienced optimisation specialists and a medium- to long-term connection to the generator project.

HEP experiments, which are now managed by very large collaborations including many technical experts, can also play a key role in sustaining a healthy relationship between theory and experiment software. The effort to work on common tools that benefit both the experiment itself and the wider community would provide shared value that justifies direct investment from the stakeholders. This model would also be beneficial for core HEP tools like LHAPDF, HepMC and Rivet, where future improvements have no theoretical physics interest anymore, putting them in a similar situation to generator performance improvements. One structural issue blocking such a mode of operation is that some experiments do not currently recognise contributions to external projects as experiment service work—a situation deserving of review in areas where external software tools are critical to experiment success.

In the following, we describe specific areas of R&D for event generation up to 2022 and beyond.

- The development of new and improved theoretical algorithms provides the largest potential for improving event generators. While it is not guaranteed that simply increasing the effort dedicated to this task will bring about the desired result, the long-term support of event generator development, and the creation of career opportunities in this research area, are critical given the commitment to experiments on multi-decade scales.
- Expand development in reweighting event samples, where new physics signatures can be explored by updating the partonic weights according to new matrix elements. It is necessary that the phase space for the updated model be a subset of the original one, which is an important limitation. The procedure is more complex at NLO and can require additional information to be stored in the event files to properly reweight in different cases. Overcoming the technical issues from utilising negative event weights is crucial. Nevertheless, the method can be powerful in many cases, and would hugely reduce the time needed for the generation of BSM samples.
- At a more technical level, concurrency is an avenue that has yet to be explored in depth for event generation. As the calculation of matrix elements requires VEGAS-style integration, this work would be helped by the development of a new Monte-Carlo integrator. For multi-particle interactions, factorising the full phase space integration into lower dimensional integrals would be a powerful method of parallelising, while the interference between different Feynman graphs can be handled with known techniques.
- For many widely used generators, basic problems of concurrency and thread hostility need to be tackled, to make these packages suitable for efficient large-scale use on modern processors and within modern HEP software frameworks. Providing appropriate common tools for interfacing, benchmarking and optimising multithreaded code would allow expertise to be shared effectively [48].
- In most generators, parallelism was added post-facto, which leads to scaling problems when the level of parallelism becomes very large, e.g., on HPC machines. These HPC machines will be part of the computing resource pool used by HEP, so solving scaling issues on these resources for event generation is important, particularly as the smaller generator code bases can make porting to non-x86_64 architectures more tractable. The problem of long and inefficient initialisation when a job utilises hundreds or thousands of cores on an HPC needs to be

tackled. While the memory consumption of event generators is generally modest, the generation of tree-level contributions to high multiplicity final states can use significant memory, and gains would be expected from optimising here.
- An underexplored avenue is the efficiency of event generation as used by the experiments. An increasingly common usage is to generate very large inclusive event samples, which are filtered on event final-state criteria to decide which events are to be retained and passed onto detector simulation and reconstruction. This naturally introduces a large waste of very CPU-expensive event generation, which could be reduced by developing filtering tools within the generators themselves, designed for compatibility with the experiments' requirements. A particularly wasteful example is where events are separated into orthogonal subsamples by filtering, in which case the same large inclusive sample is generated many times, with each stream filtering the events into a different group: allowing a single inclusive event generation to be filtered into several orthogonal output streams would improve efficiency.

Detector Simulation

Scope and Challenges

For all its success so far, the challenges faced by the HEP field in the simulation domain are daunting. During the first two runs, the LHC experiments produced, reconstructed, stored, transferred, and analysed tens of billions of simulated events. This effort required more than half of the total computing resources allocated to the experiments. As part of the HL-LHC physics programme, the upgraded experiments expect to collect 150 times more data than in Run 1; demand for larger simulation samples to satisfy analysis needs will grow accordingly. In addition, simulation tools have to serve diverse communities, including accelerator-based particle physics research utilising proton–proton colliders, neutrino, dark matter, and muon experiments, as well as the cosmic frontier. The complex detectors of the future, with different module- or cell-level shapes, finer segmentation, and novel materials and detection techniques, require additional features in geometry tools and bring new demands on physics coverage and accuracy within the constraints of the available computing budget. The diversification of the physics programmes also requires new and improved physics models. More extensive use of Fast Simulation is a potential solution, under the assumption that it is possible to improve time performance without an unacceptable loss of physics accuracy.

The gains that can be made by speeding up critical elements of the Geant4 simulation toolkit can be leveraged for all applications that use it, and it is, therefore, well worth the investment in effort needed to achieve it. The main challenges to be addressed if the required physics and software performance goals are to be achieved are:

- Review the implementations of physics models, including the assumptions, approximations, and limitations. In the best cases this can achieve higher precision and improve runtime performance through code modernisation [99]. The extension of the validity of models up to energies of 100 TeV is foreseen for the Future Circular Collider (FCC) project [141] and provides a good opportunity for this modernisation.
- Redesigning, developing, and commissioning detector simulation toolkits to be more efficient when executed on current vector CPUs and emerging new architectures, including GPUs, where use of SIMD vectorisation is vital; this includes porting and optimising the experiments' simulation applications to allow exploitation of large HPC facilities.
- Exploring different fast simulation options, where the full detector simulation is replaced, in whole or in part, by computationally efficient techniques. An area of investigation is common frameworks for fast tuning and validation.
- Developing, improving and optimising geometry tools that can be shared among experiments to make the modeling of complex detectors computationally more efficient, modular, and transparent.
- Developing techniques for background modeling, including contributions of multiple hard interactions overlapping the event of interest in collider experiments (pileup).
- Revisiting digitisation algorithms to improve performance and exploring opportunities for code sharing among experiments.

It is obviously of critical importance that the whole community of scientists working in the simulation domain continue to work together in as efficient a way as possible to deliver the required improvements. Very specific expertise is required across all simulation domains, such as physics modeling, tracking through complex geometries and magnetic fields, and building realistic applications that accurately simulate highly complex detectors. Continuous support is needed to recruit, train, and retain people with a unique set of skills needed to guarantee the development, maintenance, and support of simulation codes over the long timeframes foreseen in the HEP experimental programme.

Current Practices

The Geant4 detector simulation toolkit is at the core of simulation in almost every HEP experiment. Its continuous development, maintenance, and support for the experiments is of vital importance. New or refined functionality in physics coverage and accuracy continues to be delivered in the ongoing development programme and software performance improvements are introduced whenever possible.

Physics models are a critical part of the detector simulation, and are continuously being reviewed, and in some cases reimplemented, in order to improve accuracy and software performance. Electromagnetic (EM) transport simulation is challenging as it occupies a large part of the computing resources used in full detector simulation. Significant efforts have been made in the recent past to better describe the simulation of electromagnetic shower shapes, in particular to model the $H \rightarrow \gamma\gamma$ signal and background accurately at the LHC. This effort is being continued with an emphasis on reviewing the models' assumptions, approximations, and limitations, especially at very high energy, with a view to improving their respective software implementations. In addition, a new "theory-based" model (Goudsmit–Saunderson), for describing the multiple scattering of electrons and positrons, has been developed that has been demonstrated to outperform, in terms of physics accuracy and speed, the current models in Geant4. The models used to describe the bremsstrahlung process have also been reviewed, and recently an improved theoretical description of the Landau–Pomeranchuk–Migdal effect was introduced that plays a significant role at high energies. Theoretical review of all electromagnetic models, including those of hadrons and ions, is therefore, of high priority both for HL-LHC and for FCC studies.

Hadronic physics simulation covers purely hadronic interactions. It is not possible for a single model to describe all the physics encountered in a simulation due to the large energy range that needs to be covered and the simplified approximations that are used to overcome the difficulty of solving the full theory (QCD). Currently the most-used reference physics list for high energy and space applications is FTFP_BERT. It uses the Geant4 Bertini cascade for hadron–nucleus interactions from 0 to 12 GeV incident hadron energy and the FTF parton string model for hadron–nucleus interactions from 3 GeV upwards. QGSP_BERT is a popular alternative which replaces the FTF model with the QGS model over the high energy range. The existence of more than one model (for each energy range) is very valuable to be able to determine the systematics effects related to the approximations used. The use of highly granular calorimeters, such as the ones being designed by the CALICE collaboration for future linear colliders, allows a detailed validation of the development of hadronic showers with test-beam data. Preliminary results suggest that the lateral profiles of Geant4 hadronic showers are too narrow. Comparisons with LHC test-beam data have shown that a fundamental ingredient for improving the description of the lateral development of showers is the use of intermediate and low energy models that can describe the cascading of hadrons in nuclear matter. Additional work is currently being invested in the further improvement of the QGS model, which is a more theory-based approach than the phenomenological FTF model, and therefore, offers better confidence at high energies, up to a few TeV. This again is a large endeavour and requires continuous effort over a long time.

The Geant4 collaboration is working closely with user communities to enrich the physics models' validation system with data acquired during physics runs and test beam campaigns. In producing new models of physics interactions and improving the fidelity of the models that exist, it is absolutely imperative that high-quality data are available. Simulation model tuning often relies on test beam data, and a program to improve the library of available data could be invaluable to the community. Such data would ideally include both thin-target test beams for improving interaction models and calorimeter targets for improving shower models. This data could potentially be used for directly tuning Fast Simulation models as well.

There are specific challenges associated with the Intensity Frontier experimental programme, in particular simulation of the beamline and the neutrino flux. Neutrino experiments rely heavily on detector simulations to reconstruct neutrino energy, which requires accurate modelling of energy deposition by a variety of particles across a range of energies. Muon experiments such as Muon g-2 and Mu2e also face large simulation challenges; since they are searching for extremely rare effects, they must grapple with very low signal to background ratios and the modeling of low cross-section background processes. Additionally, the size of the computational problem is a serious challenge, as large simulation runs are required to adequately sample all relevant areas of experimental phase space, even when techniques to minimise the required computations are used. There is also a need to simulate the effects of low energy neutrons, which requires large computational resources. Geant4 is the primary simulation toolkit for all of these experiments.

Simulation toolkits do not include effects like charge drift in an electric field or models of the readout electronics of the experiments. Instead, these effects are normally taken into account in a separate step called digitisation. Digitisation is inherently local to a given sub-detector and often even to a given readout element, so that there are many opportunities for parallelism in terms of vectorisation and multiprocessing or multithreading, if the code and the data objects are designed optimally. Recently, both hardware and software projects have benefitted from an increased level of sharing among experiments. The LArSoft Collaboration develops and supports a shared base of physics software across Liquid Argon (LAr) Time Projection Chamber (TPC) experiments, which includes providing common digitisation code. Similarly, an effort exists among the LHC experiments to share code for modeling radiation damage effects in silicon. As ATLAS and CMS expect to use similar readout chips in their future trackers, further code sharing might be possible.

The Geant4 simulation toolkit will also evolve over the next decade to include contributions from various R&D projects, as described in the following section. This is required to ensure the support of experiments through continuous maintenance and improvement of the Geant4 simulation toolkit. This is necessary until production versions of potentially alternative engines, such as those resulting from ongoing R&D work, become available, integrated, and validated by experiments. The agreed ongoing strategy to make this adoption possible is to ensure that new developments resulting from the R&D programme can be tested with realistic prototypes and then be integrated, validated, and deployed in a timely fashion in Geant4.

Research and Development Programme

To meet the challenge of improving the performance by a large factor, an ambitious R&D programme is underway to investigate each component of the simulation software for the long term. In the following we describe in detail some of the studies to be performed in the next 3–5 years.

- Particle transport and vectorisation: the study of an efficient transport of particles (tracks) in groups so as to maximise the benefit of using SIMD operations.
- Modularisation: improvement of Geant4 design to allow for a tighter and easier integration of single sub-packages of the code into experimental frameworks.
- Physics models: extensions and refinements of the physics algorithms to provide new and more performant physics capabilities.
- Other activities: integration of multi-threading capabilities in experiment applications; experiment-agnostic software products to cope with increased pileup, fast simulation, digitisation, and efficient production of high-quality random numbers.

Particle transport and vectorisation One of the most ambitious elements of the simulation R&D programme is a new approach to managing particle transport, which has been introduced by the GeantV project. The aim is to deliver a multithreaded vectorised transport engine that has the potential to deliver large performance benefits. Its main feature is track-level parallelisation, bundling particles with similar properties from different events to process them in a single thread. This approach, combined with SIMD vectorisation coding techniques and improved data locality, is expected to yield significant speed-ups, which are to be measured in a realistic prototype currently under development. For the GeantV transport engine to display its best computing performance, it is necessary to vectorise and optimise the accompanying modules, including geometry, navigation, and the physics models. These are developed as independent libraries so that they can also be used together with the current Geant4 transport engine. Of course, when used with the current Geant4 they will not expose their full performance potential, since transport in Geant4 is currently sequential, but this allows for a preliminary validation and comparison with the existing implementations. The benefit of this approach is that new developments can be delivered as soon as they are available. The new Vectorised Geometry package (VecGeom), developed as part of GeantV R&D and successfully integrated into Geant4, is an example that demonstrated the benefit of this approach. By the end of 2018 it is intended to have a proof-of-concept for the new particle transport engine that includes vectorised EM physics, vectorised magnetic field propagation and that uses the new vectorised geometry package. This will form a sound basis for making performance comparisons for simulating EM showers in a realistic detector.

- 2019: the *beta* release of the GeantV transport engine will contain enough functionality to build the first real applications. This will allow performance to be measured and give sufficient time to prepare for HL-LHC running. It should include the use of vectorisation in most of the components, including physics modelling for electrons, gammas and positrons, whilst still maintaining simulation reproducibility, and I/O in a concurrent environment and multi-event user data management.

Modularisation Starting from the next release, a modularisation of Geant4 is being pursued that will allow an easier integration in experimental frameworks, with the possibility to include only the Geant4 modules that are actually used. A further use case is the possibility to use one of the Geant4 components in isolation, e.g., to use hadronic interaction modeling without kernel components from a fast simulation framework. As a first step a preliminary review of libraries' granularity is being pursued, which will be followed by a review of intra-library dependencies with the final goal of reducing their dependencies.

- 2019: Redesign of some Geant4 kernel components to improve the efficiency of the simulation on HPC systems, starting from improved handling of Geant4 *database*s on large core-count systems. A review will be made of the multithreading design to be closer to task-based frameworks, such as Intel's Threaded Building Blocks (TBB) [79].

Physics models It is intended to develop new and extended physics models to cover extended energy and physics processing of present and future colliders, Intensity Frontier experiments, and direct dark matter search experiments. The goal is to extend the missing models (e.g., neutrino interactions), improve models' physics accuracy and, at the same time, improve CPU and memory efficiency. The deliverables of these R&D efforts include physics modules that produce equivalent quality physics, and will therefore, require extensive validation in realistic applications.

- 2020: Improved implementation of hadronic cascade models for LHC and, in particular, Liquid Argon detectors. Improved accuracy models of EM interactions of photons and electrons. To address the needs of cosmic frontier experiments, optical photon transport must be improved and made faster.
- 2022: Implementation of EPOS string model for multi-GeV to multi-TeV interactions, for FCC detector simulation and systematic studies of HL-LHC detectors.

Experiment applications The experiment applications are essential for validating the software and physics performance of new versions of the simulation toolkit. ATLAS and CMS have already started to integrate Geant4 multithreading capability in their simulation applications; in the case of CMS the first Full Simulation production in multithreaded mode was delivered in the autumn of 2017. Specific milestones are as follows:

- 2020: LHC, Neutrino, Dark Matter, and Muon experiments to demonstrate the ability to run their detector simulation in multithreaded mode, using the improved navigation and electromagnetic physics packages. This should bring experiments more accurate physics and improved performance.
- 2020: Early integration of the beta release of the GeantV transport engine in the experiments' simulation, including the implementation of the new user interfaces, which will allow the first performance measurements and physics validation to be made.
- 2022: The availability of a production version of the new track-level parallelisation and fully vectorised geometry, navigation, and physics libraries will offer the experiments the option to finalise integration into their frameworks; intensive work will be needed in physics validation and computing performance tests. If successful, the new engine could be in production on the timescale of the start of the HL-LHC run in 2026.

Pileup Backgrounds to hard-scatter events have many components including in-time pileup, out-of-time pileup, cavern background and beam-gas collisions. All of these components can be simulated, but they present storage and I/O challenges related to the handling of the large simulated minimum bias samples used to model the extra interactions. An R&D programme is needed to study different approaches to managing these backgrounds within the next 3 years:

- Real zero-bias events can be collected, bypassing any zero suppression, and overlaid on the fully simulated hard scatters. This approach faces challenges related to the collection of non-zero-suppressed samples or the use of suppressed events, non-linear effects when adding electronic signals from different samples, and sub-detector misalignment consistency between the simulation and the real experiment. Collecting calibration and alignment data at the start of a new Run would necessarily incur delays such that this approach is mainly of use in the final analyses. The experiments are expected to invest in the development of the zero-bias overlay approach by 2020.
- The baseline option is to "pre-mix" together the minimum bias collisions into individual events that have the full background expected for a single collision of interest. Experiments will invest effort on improving their premixing techniques, which allow the mixing to be performed at the digitisation level, reducing the disk and network usage for a single event.

Fast simulation The work on Fast Simulation is also accelerating with the objective of producing a flexible framework that permits Full and Fast simulation to be combined for different particles in the same event. Various approaches to Fast Simulation are being tried all with the same goal of saving computing time, under the assumption that it is possible to improve time performance without an unacceptable loss of physics accuracy. There has recently been a great deal of interest in the use of Machine Learning in Fast Simulation, most of which has focused on the use of multi-objective regression and Generative Adversarial Networks (GANs) [70]. Since use of GANs allows for non-parametric learning in cases such as calorimetric shower fluctuations, it is a promising avenue for generating non-Gaussian and highly correlated physical effects. This is an obvious area for future expansion and development, as it is currently in its infancy.

- 2018: Assessment of the benefit of machine learning approach for fast simulation.
- 2019: ML-based Fast Simulation for some physics observables.
- 2022: Demonstrate the potential of a common Fast Simulation infrastructure applicable to the variety of detector configurations.

Digitisation It is expected that, within the next 3 years, common digitisation efforts are well-established among experiments, and advanced high-performance generic digitisation examples, which experiments could use as a basis to develop their own code, become available. For example, the development of next generation silicon detectors requires realistic simulation of the charge collection and digitisation processes. Owing to the large variety of technologies, common software frameworks need to be flexible and modular to cater for the different needs.

- 2020: Deliver advanced high-performance, SIMD-friendly generic digitisation examples that experiments can use as a basis to develop their own code.
- 2022: Fully tested and validated optimised digitisation code that can be used by the HL-LHC and DUNE experiments.

Pseudorandom number generation The selection of Pseudorandom Number Generators (PRNGs) presents challenges when running on infrastructures with a large degree of parallelism, as reproducibility is a key requirement. HEP will collaborate with researchers in the development of PRNGs, seeking to obtain generators that address better our challenging requirements. Specific milestones are:

- 2020: Develop a single library containing sequential and vectorised implementations of the set of state-of-the-art PRNGs, to replace the existing ROOT and CLHEP implementations. Potential use of C++11 PRNG interfaces and implementations, and their extension for our further requirements (output of multiple values, vectorisation) will be investigated.
- 2022: Promote a transition to the use of this library to replace existing implementations in ROOT and Geant4.

Software Trigger and Event Reconstruction

Scope and Challenges

The reconstruction of raw detector data and simulated data, and its processing in real time, represent a major component of today's computing requirements in HEP. Advances in the capabilities of facilities and future experiments bring the potential for a dramatic increase in physics reach, at the price of increased event complexities and rates. It is, therefore, essential that event reconstruction algorithms and software triggers continue to evolve so that they are able to efficiently exploit future computing architectures, and deal with the increase in data rates without loss of physics. Projections into future, e.g., at HL-LHC conditions, show that without significant changes in approach or algorithms the increase in resources needed would be incompatible with the expected budget.

At the HL-LHC, the central challenge for object reconstruction is to maintain excellent efficiency and resolution in the face of high pileup values, especially at low transverse momentum (p_{T}). Detector upgrades, such as increases in channel density, high-precision timing, and improved detector geometric layouts, are essential to overcome these problems. In many cases these new technologies bring novel requirements to software trigger and/or event reconstruction algorithms, or require new algorithms to be developed. Ones of particular importance at the HL-LHC include high-granularity calorimetry, precision timing detectors, and hardware triggers based on tracking information, which may seed later software trigger and reconstruction algorithms.

At the same time, trigger systems for next-generation experiments are evolving to be more capable, both in their ability to select a wider range of events of interest for the physics programme, and their ability to stream a larger rate of events for further processing. ATLAS and CMS both target systems where the output of the hardware trigger system is increased by an order of magnitude over the current capability, up to 1 MHz [15, 45]. In LHCb [90] and ALICE [30], the full collision rate (between 30 and 40 MHz for typical LHC proton–proton operations) will be streamed to real-time or near-real-time software trigger systems. The increase in event complexity also brings a "problem" of an overabundance of signals to the experiments, and specifically to the software trigger algorithms. The evolution towards a genuine real-time analysis of data has been driven by the need to analyse more signal than can be written out for traditional processing, and technological developments that enable this without reducing the analysis sensitivity or introducing biases.

Evolutions in computing technologies are an opportunity to move beyond commodity x86_64 technologies, which HEP has used very effectively over the past 20 years, but also represent a significant challenge if we are to derive sufficient event processing throughput per cost to reasonably enable our physics programmes [26]. Among these challenges, important items identified include the increase of SIMD capabilities, the evolution towards multi- or many-core architectures, the slow increase in memory bandwidth relative to CPU capabilities, the rise of heterogeneous hardware, and the possible evolution in facilities available to HEP production systems.

The move towards open source software development and continuous integration systems brings opportunities to assist developers of software trigger and event reconstruction algorithms. Continuous integration systems based on standard open-source tools have already allowed automated code quality and performance checks, both for algorithm developers and code integration teams. Scaling these up to allow for sufficiently high-statistics checks is still an outstanding challenge. Also, code quality demands increase as traditional offline analysis components migrate into trigger systems, where algorithms can only be run once, and any problem means losing data permanently.

Current Practices

Substantial computing facilities are in use for both online and offline event processing across all experiments surveyed. In most experiments, online facilities are dedicated to the operation of the software trigger, but a recent trend has been to use them opportunistically for offline processing too, when the software trigger does not make them 100% busy. On the other hand, offline facilities are shared with event reconstruction, simulation, and analysis. CPU in use by experiments is typically measured at the scale of tens or hundreds of thousands of x86_64 processing cores.

The CPU needed for event reconstruction tends to be dominated by charged particle reconstruction (tracking), especially when the number of collisions per bunch crossing is high and an efficient reconstruction low p_T particles is required. Calorimetric reconstruction, particle flow reconstruction, and particle identification algorithms also make up significant parts of the CPU budget in some experiments. Disk storage is typically 10s to 100s of PBs per experiment. It is dominantly used to make the output of the event reconstruction, both for real data and simulation, available for analysis.

Current experiments have moved towards smaller, but still flexible, tiered data formats. These tiers are typically based on the ROOT file format and constructed to facilitate both skimming of interesting events and the selection of interesting pieces of events by individual analysis groups or through centralised analysis processing systems. Initial implementations of real-time analysis systems are in use within several experiments. These approaches remove the detector data that typically makes up the raw data tier kept for offline reconstruction, and keep only final analysis objects [3, 85, 155].

Systems critical for reconstruction, calibration, and alignment generally implement a high level of automation in all experiments. They are an integral part of the data taking and data reconstruction processing chain, both in the online systems as well as the offline processing setup.

Research and Development Programme

Seven key areas, itemised below, have been identified where research and development is necessary to enable the community to exploit the full power of the enormous datasets that we will be collecting. Three of these areas concern the increasingly parallel and heterogeneous computing architectures that we will have to write our code for. In addition to a general effort to vectorise our codebases, we must understand what kinds of algorithms are best suited to what kinds of hardware architectures. It is an area where collaboration with the computer science community is required. We also need to develop benchmarks that allow us to compare the physics-per-dollar-per-watt performance of different algorithms across a range of potential architectures, and find ways to optimally utilise heterogeneous processing centres. The consequent increase in the complexity and diversity of our codebase will necessitate both a determined push to educate physicists in modern algorithmic approaches and coding practices, and a development of more sophisticated and automated quality assurance and control. The increasing granularity of our detectors, and the addition of timing information, which seems mandatory to cope with the extreme pileup conditions at the HL-LHC, will require new kinds of reconstruction algorithms that are sufficiently fast for use in real-time. Finally, the increased signal rates will mandate a push towards real-time analysis in many areas of HEP, in particular those with low-p_T signatures.

- HEP developed toolkits and algorithms typically make poor use of vector units on commodity computing systems. Improving this will bring speedups to applications running on both current computing systems and most future architectures. The goal for work in this area is to evolve current toolkit and algorithm implementations, and best programming techniques, to better use SIMD capabilities of current and future CPU architectures.
- Computing platforms are generally evolving towards having more cores to increase processing capability. This evolution has resulted in multithreaded frameworks in use, or in development, across HEP. Algorithm developers can improve throughput by being thread-safe and enabling the use of fine-grained parallelism. The goal is to evolve current event models, toolkits and algorithm implementations, and best programming techniques, to improve the throughput of multithreaded software trigger and event reconstruction applications.
- Computing architectures using technologies beyond CPUs offer an interesting alternative for increasing throughput of the most time-consuming trigger or reconstruction algorithms. Examples such as GPUs and FPGAs could be integrated into dedicated trigger or specialised reconstruction processing facilities, in particular online computing farms. The goal is to demonstrate how the throughput of toolkits or algorithms can be improved in a production environment and to understand how much these new architectures require rethinking the algorithms used today. In addition, it is necessary to assess and minimise possible additional costs coming from the maintenance of multiple implementations of the same algorithm on different architectures.
- HEP experiments have extensive continuous integration systems, including varying code regression checks that have enhanced the Quality Assurance (QA) and Quality Control (QC) procedures for software development in recent years. These are typically maintained by individual experiments and have not yet reached the point where

statistical regression, technical, and physics performance checks can be performed for each proposed software change. The goal is to enable the development, automation, and deployment of extended QA and QC tools and facilities for software trigger and event reconstruction algorithms.
- Real-time analysis techniques are being adopted to enable a wider range of physics signals to be saved by the trigger for final analysis. As rates increase, these techniques can become more important and widespread by enabling only the parts of an event associated with the signal candidates to be saved, reducing the disk space requirement. The goal is to evaluate and demonstrate the tools needed to facilitate real-time analysis techniques. Research topics include the study of compression and custom data formats, toolkits for real-time detector calibration and validation that enable full offline analysis chains to be ported into real-time, and frameworks that allow non-expert offline analysts to design and deploy real-time analyses without compromising data taking quality.
- The central challenge for object reconstruction at the HL-LHC is to maintain excellent efficiency and resolution in the face of high pileup, especially at low object p_T. Trigger systems and reconstruction software need to exploit new techniques and higher granularity detectors to maintain or even improve physics measurements in the future. It is also becoming increasingly clear that reconstruction in very high pileup environments, such as the HL-LHC or FCC-hh, will not be possible without adding some timing information to our detectors, to exploit the finite time during which the beams cross and the interactions are produced. The goal is to develop and demonstrate efficient techniques for physics object reconstruction and identification in complex environments.
- Future experimental facilities will bring a large increase in event complexity. The performance scaling of current-generation algorithms with this complexity must be improved to avoid a large increase in resource needs. In addition, it may become necessary to deploy new algorithms to solve these problems, including advanced machine learning techniques. The goal is to evolve or rewrite existing toolkits and algorithms focused on their physics and technical performance at high event complexity, e.g., high pileup at HL-LHC. Most important targets are those which limit expected throughput performance at future facilities, most significantly charged-particle tracking. A number of efforts in this area are already in progress [9].

Data Analysis and Interpretation

Scope and Challenges

Scientific questions are answered by analysing the data obtained from suitably designed experiments and comparing measurements with predictions from models and theories. Such comparisons are typically performed long after data taking, but can sometimes also be executed in near-real time on selected samples of reduced size.

The final stages of analysis are undertaken by small groups or even individual researchers. The baseline analysis model utilises successive stages of data reduction, finally reaching a compact dataset for quick real-time iterations. This approach aims at exploiting the maximum possible scientific potential of the data, whilst minimising the "time to insight" for a large number of different analyses performed in parallel. It is a complicated combination of diverse criteria, ranging from the need to make efficient use of computing resources to the management styles of the experiment collaborations. Any analysis system has to be flexible enough to cope with deadlines imposed by conference schedules. Future analysis models must adapt to the massive increases in data taken by the experiments, while retaining this essential "time to insight" optimisation.

Over the past 20 years the HEP community has developed and gravitated around a single analysis ecosystem based on ROOT.

ROOT is a general-purpose object-oriented framework that addresses the selection, integration, development, and support of a number of foundation and utility class libraries that can be used as a basis for developing HEP application codes. The added value to the HEP community is that it provides an integrated and validated toolkit, and its use encompasses the full event processing chain; it has a major impact on the way HEP analysis is performed. This lowers the hurdle to start an analysis, enabling the community to communicate using a common analysis language, as well as making common improvements as additions to the toolkit quickly become available. The ongoing ROOT programme of work addresses important new requirements, in both functionality and performance, and this is given a high priority by the HEP community.

An important new development in the analysis domain has been the emergence of new analysis tools coming from industry and open-source projects (e.g. Jupyter notebooks [83], the scikit-learn package [107]), and this presents new opportunities for improving the HEP analysis software ecosystem. The HEP community is very interested in using these software tools, together with established components, in an interchangeable way. The main challenge will be to enable new open-source tools to be plugged in dynamically to the existing ecosystem and to provide mechanisms that allow the existing and new components to interact and exchange data efficiently. To improve our ability to analyse much larger datasets, R&D will be needed to investigate file formats, compression algorithms, and new ways of storing and accessing data for analysis and to adapt workflows to run on future computing infrastructures.

Reproducibility is the cornerstone of scientific results. It is currently difficult to repeat most HEP analyses in exactly the manner they were originally performed. This difficulty mainly arises due to the number of scientists involved, the large number of steps in a typical HEP analysis workflow, and the complexity of the analyses themselves. A challenge specific to data analysis and interpretation is tracking the evolution of relationships between all the different components of an analysis, i.e. the provenance of each step.

Reproducibility of scientific results goes in hand with the need to preserve both the data and the software. "Data and software preservation" develops this latter topic where the FAIR principles of data management are embraced.

Robust methods for data reinterpretation are also critical. Collaborations typically interpret results in the context of specific models for new physics searches and sometimes reinterpret those same searches in the context of alternative theories. However, understanding the full implications of these searches requires the interpretation of the experimental results in the context of many more theoretical models that are currently explored at the time of publication. Analysis reproducibility and reinterpretation strategies need to be considered in all new approaches under investigation, so that they become a fundamental component of the system as a whole.

Adapting to the rapidly evolving landscape of software tools, as well as to methodological approaches to data analysis, requires effort in continuous training, both for novices as well as for experienced researchers, as detailed in "Training and careers". The maintenance and sustainability of the current analysis ecosystem also present a major challenge, as currently this effort is provided by just a few institutions. Legacy and less-used parts of the ecosystem need to be managed appropriately. New policies are needed to retire little used or obsolete components and free up effort for the development of new components. These new tools should be made attractive and useful to a significant part of the community to attract new contributors.

Current Practices

Methods for analysing HEP data have been developed over many years and successfully applied to produce physics results, including more than 2000 publications, during LHC Runs 1 and 2. Analysis at the LHC experiments typically starts with users running code over centrally managed data that is of O (100 kB/event) and contains all of the information required to perform a typical analysis leading to publication. The most common approach is through a campaign of data reduction and refinement, ultimately producing simplified data structures of arrays of simple data types ("flat ntuples") and histograms used to make plots and tables, from which physics results can be derived.

The current centrally managed data typically used by a Run 2 data analysis at the LHC (hundreds of TB) is far too large to be delivered locally to the user. An often-stated requirement of the data reduction steps is to arrive at a dataset that "can fit on a laptop", to facilitate low-latency, high-rate access to a manageable amount of data during the final stages of an analysis. Creating and retaining intermediate datasets produced by data reduction campaigns, bringing and keeping them "close" to the analysers, is designed to minimise latency and the risks related to resource contention. At the same time, disk space requirements are usually a key constraint of the experiment computing models. The LHC experiments have made a continuous effort to produce optimised analysis-oriented data formats with enough information to avoid the need to use intermediate formats. Another effective strategy has been to combine analyses from different users and execute them within the same batch jobs (the so-called "analysis trains"), thereby reducing the number of times data must be read from the storage systems. This has improved performance and usability, and simplified the task of the bookkeeping.

There has been a huge investment in using C++ for performance-critical code, in particular in event reconstruction and simulation, and this will continue in the future. However, for analysis applications, Python has emerged as the language of choice in the data science community, and its use continues to grow within HEP. Python is highly appreciated for its ability to support fast development cycles, for its ease-of-use, and it offers an abundance of well-maintained and advanced open source software packages. Experience shows that the simpler interfaces and code constructs of Python could reduce the complexity of analysis code, and therefore contribute to decreasing the "time to insight" for HEP analyses, as well as increasing their sustainability. Increased HEP investment is needed to allow Python to become a first-class supported language.

One new model of data analysis, developed outside of HEP, maintains the concept of sequential reduction, but mixes interactivity with batch processing. These exploit new cluster management systems, most notably Apache Spark [11, 12], which uses open-source tools contributed both by industry and the data-science community. Other products implementing the same analysis concepts and workflows are emerging, such as TensorFlow [96], Dask [51, 115], Pachyderm [134], Blaze [156], Parsl [17], and Thrill [24]. This approach can complement the present and widely adopted Grid processing of datasets. It may potentially simplify the access to data and the expression of parallelism, thereby improving the exploitation of cluster resources.

An alternative approach, which was pioneered in astronomy but has become more widespread throughout the Big Data world, is to perform fast querying of centrally managed data and compute remotely on the queried data to produce the analysis products of interest. The analysis workflow is accomplished without focus on persistence of data traditionally associated with data reduction, although transient data may be generated to efficiently accomplish this workflow and optionally can be retained to facilitate an analysis "checkpoint" for subsequent execution. In this approach, the focus is on obtaining the analysis end-products in a way that does not necessitate a data reduction campaign. It is of interest to understand the role that such an approach could have in the global analysis infrastructure, and if it can bring an optimisation of the global storage and computing resources required for the processing of raw data to analysis.

Another active area regarding analysis in the world outside HEP is the switch to a functional or declarative programming model, as for example provided by Scala [153] in the Spark environment. This allows scientists to express the intended data transformation as a query on data. Instead of having to define and control the "how", the analyst declares the "what" of their analysis, essentially removing the need to define the event loop in an analysis, and leave it to underlying services and systems to optimally iterate over events. It appears that these high-level approaches will allow abstraction from the underlying implementations, allowing the computing systems more freedom in optimising the utilisation of diverse forms of computing resources. R&D is already under way, e.g., TDataFrame [73] in ROOT, and this needs to be continued with the ultimate goal of establishing a prototype functional or declarative programming paradigm.

Research and Development Programme

Towards HL-LHC, we envisage dedicated data analysis facilities for experimenters, offering an extendable environment that can provide fully functional analysis capabilities, integrating all these technologies relevant for HEP. Initial prototypes of such analysis facilities are currently under development. On the time scale of HL-LHC, such dedicated analysis facilities would provide a complete system engineered for latency optimisation and stability.

The following R&D programme lists the tasks that need to be accomplished. By 2020:

- Enable new open-source software tools to be plugged in dynamically to the existing ecosystem, and provide mechanisms to dynamically exchange parts of the ecosystem with new components.
- Prototype a comprehensive set of mechanisms for interacting and exchanging data between new open-source tools and the existing analysis ecosystem.
- Complete an advanced prototype of a low-latency response, high-capacity analysis facility, incorporating fast caching technologies to explore a query-based analysis approach and open-source cluster-management tools. It should, in particular, include an evaluation of additional storage layers, such as SSD storage and NVRAM-like storage, and cloud and Big Data orchestration systems.
- Expand support of Python in our ecosystem with a strategy for ensuring long-term maintenance and sustainability. In particular in ROOT, the current Python bindings should evolve to reach the ease of use of native Python modules.
- Develop a prototype based on a functional or declarative programming model for data analysis.
- Conceptualise and prototype an analysis "Interpretation Gateway", including data repositories, e.g., HEPData [77, 93], and analysis preservation and reinterpretation tools.

By 2022:

- Evaluate chosen architectures for analysis facilities, verify their design and provide input for corrective actions to test them on a larger scale during Run 3.
- Develop a blueprint for remaining analysis facility developments, system design and support model.

Machine Learning

Machine Learning (ML) is a rapidly evolving approach to characterising and describing data with the potential to radically change how data is reduced and analysed. Some applications will qualitatively improve the physics reach of datasets. Others will allow much more efficient use of processing and storage resources, effectively extending the physics reach of experiments. Many of the activities in this area will explicitly overlap with those in the other focus areas, whereas others will be more generic. As a first approximation, the HEP community will build domain-specific applications on top of existing toolkits and ML algorithms developed by computer scientists, data scientists, and scientific software developers from outside the HEP world. Work will also be done to understand where problems do not map well onto existing paradigms and how these problems can be recast into abstract formulations of more general interest.

Scope and Challenges

The Machine Learning, Statistics, and Data Science communities have developed a variety of powerful ML approaches for classification (using pre-defined categories), clustering (where categories are discovered), regression (to produce continuous outputs), density estimation, dimensionality reduction, etc. Some of these have been used productively in HEP for more than 20 years, others have been introduced relatively recently. The portfolio of ML techniques and tools is in constant evolution, and a benefit is that many have well-documented open source software implementations. ML has already become ubiquitous in some HEP applications, most notably in classifiers used to discriminate between signals and backgrounds in final offline analyses. It is also increasingly used in both online and offline reconstruction and particle identification algorithms, as well as the classification of reconstruction-level objects, such as jets.

The abundance of, and advancements in, ML algorithms and implementations present both opportunities and challenges for HEP. The community needs to understand which are most appropriate for our use, tradeoffs for using one tool compared to another, and the tradeoffs of using ML algorithms compared to using more traditional software. These issues are not necessarily "factorisable", and a key goal will be to ensure that, as HEP research teams investigate the numerous approaches at hand, the expertise acquired and lessons learned, get adequately disseminated to the wider community. In general, each team, typically a small group of scientists from a collaboration, will serve as a source of expertise, helping others develop and deploy experiment-specific ML-based algorithms in their software stacks. It should provide training to those developing new ML-based algorithms, as well as those planning to use established ML tools.

With the advent of more powerful hardware, particularly GPUs and ML dedicated processors, as well as more performant ML algorithms, the ML toolset will be used to develop application software that could potentially, amongst other things:

- Replace the most computationally expensive parts of pattern recognition algorithms and parameter extraction algorithms for characterising reconstructed objects. For example, investigating how ML algorithms could improve the physics performance or execution speed of charged track and vertex reconstruction, one of the most CPU intensive elements of our current software.
- Extend the use of ML algorithms for real-time event classification and analysis, as discussed in more detail in "Software trigger and event reconstruction".
- Extend the physics reach of experiments by extending the role of ML at the analysis stage: handling data/MC or control/signal region differences, interpolating between mass points, training in a systematics-aware way, etc.
- Compress data significantly with negligible loss of fidelity in terms of physics utility.

As already discussed, many particle physics detectors produce much more data than can be moved to permanent storage. The process of reducing the size of the datasets is managed by the trigger system. ML algorithms have already been used very successfully for triggering, to rapidly characterise which events should be selected for additional consideration and eventually saved to long-term storage. In the era of the HL-LHC, the challenges will increase both quantitatively and qualitatively as the number of proton–proton collisions per bunch crossing increases. The scope of ML applications in the trigger will need to expand to tackle the challenges to come.

Current Practices

The use of ML in HEP analyses has become commonplace over the past two decades, and the most common use case has been in signal/background classification. The vast majority of HEP analyses published in recent years have used the HEP-specific software package TMVA [127] included in ROOT. Recently, however, many HEP analysts have begun migrating to non-HEP ML packages such as scikit-learn [107] and Keras [37], although these efforts have yet to result in physics publications from major collaborations. Data scientists at Yandex created a Python package that provides a consistent API to most ML packages used in HEP [110]. Packages like Spearmint [126] and scikit-optimize [118] perform Bayesian optimisation and can improve HEP Monte Carlo work.

This shift in the set of ML techniques and packages utilised is especially strong in the neutrino physics community, where new experiments such as DUNE place ML at the very heart of their reconstruction algorithms and event selection. The shift is also occurring among LHC collaborations, where ML is becoming more and more commonplace in reconstruction and real-time applications. Examples where ML has already been deployed in a limited way include charged and neutral particle reconstruction and identification, jet reconstruction and identification, and determining a particle's production properties (flavour tagging), based on information from the rest of the event. In addition, ML algorithms have been developed that are insensitive to changing detector performance, for use in real-time applications, and algorithms that are minimally biased with respect to the physical observables of interest.

At present, much of this development has happened in specific collaborations. While each experiment has, or is likely to have, different specific use cases, we expect that many of these will be sufficiently similar to each other that R&D can be done in common. Even when this is not possible, experience with one type of problem will provide insights into how to approach other types of problem. This is why the Inter-experiment Machine Learning forum (IML [81]) was created at CERN in 2016, as a compliment to experiment specific ML R&D groups. It has already fostered closer collaboration between LHC and non-LHC collaborations in the ML field.

Research and Development Roadmap and Goals

The R&D roadmap presented here is based on the preliminary work done in recent years, coordinated by the IML, which will remain the main forum to coordinate work in ML in HEP and ensure the proper links with the data science communities. The following programme of work is foreseen.

By 2020:

- *Particle identification and particle properties:* in calorimeters or Time Projection Chambers (TPCs), where the data can be represented as a 2D or 3D image (or even in 4D, including timing information), the problems can be cast as a computer vision task. Deep Learning (DL), one class of ML algorithm, in which neural networks are used to reconstruct images from pixel intensities, is a good candidate to identify particles and extract many parameters. Promising DL architectures for these tasks include convolutional, recurrent, and adversarial neural networks. A particularly important application is to Liquid Argon TPCs (LArTPCs), which is the chosen detection technology for DUNE, the new flagship experiment in the neutrino programme. A proof of concept and comparison of DL architectures should be finalised by 2020. Particle identification can also be explored to tag the flavour of jets in collider experiments (e.g., the so-called b-tagging). The investigation of these concepts, which connect to Natural Language Processing [41], has started at the LHC and is to be pursued on the same timescale.
- *ML middleware and data formats for offline usage:* HEP relies on the ROOT format for its data, whereas the ML community has developed several other formats, often associated with specific ML tools. A desirable data format for ML applications should have the following attributes: high read–write speed for efficient training, sparse readability without loading the entire dataset into RAM, compressibility, and widespread adoption by the ML community. The thorough evaluation of the different data formats and their impact on ML performance in the HEP context must be continued, and it is necessary to define a strategy for bridging or migrating HEP formats to the chosen ML format(s), or vice-versa.
- *Computing resource optimisations:* managing large volume data transfers is one of the challenges facing current computing facilities. Networks play a crucial role in data exchange and so a network-aware application layer may significantly improve experiment operations. ML is a promising technology to identify anomalies in network traffic, to predict and prevent network congestion, to detect bugs via analysis of self-learning networks, and for WAN path optimisation based on user access patterns.
- *ML as a service (MLaaS):* current cloud providers rely on a MLaaS model exploiting interactive machine learning tools to make efficient use of resources, however, this is not yet widely used in HEP. HEP services for interactive analysis, such as CERN's Service for Web-based analysis, SWAN [108], may play an important role in adoption of machine learning tools in HEP workflows. To use these tools more efficiently, sufficient and appropriately tailored hardware and instances other than SWAN will be identified.

By 2022:

- *Detector anomaly detection:* data taking is continuously monitored by physicists taking shifts to monitor and assess the quality of the incoming data, largely using reference histograms produced by experts. A whole class of ML algorithms called anomaly detection can be useful for automating this important task. Such unsupervised algorithms are able to learn from data and produce an alert when deviations are observed. By monitoring many variables at the same time, such algorithms are sensitive to subtle signs forewarning of imminent failure, so that pre-emptive maintenance can be scheduled. These techniques are already used in industry.
- *Simulation:* recent progress in high fidelity fast generative models, such as Generative Adversarial Networks (GANs) [70] and Variational Autoencoders (VAEs) [86], which are able to sample high dimensional feature distributions by learning from existing data samples, offer a promising alternative for Fast Simulation. A simplified first attempt at using such techniques in simulation saw orders of magnitude increase in speed over existing Fast Simulation techniques, but has not yet reached the required accuracy [104].
- *Triggering and real-time analysis:* one of the challenges is the trade-off in algorithm complexity and performance under strict inference time constraints. To deal with the increasing event complexity at HL-LHC, the use of sophisticated ML algorithms will be explored at all trigger levels, building on the pioneering work of the LHC collaborations. A critical part of this work will be to understand which ML techniques allow us to maximally exploit future computing architectures.
- *Sustainable Matrix Element Method (MEM):* MEM is a powerful technique that can be utilised for making measurements of physical model parameters and direct searches for new phenomena. As it is very computationally intensive its use in HEP is limited. Although the use of neural networks for numerical integration is not new, it is a technical challenge to design a network sufficiently

rich to encode the complexity of the ME calculation for a given process over the phase space relevant to the signal process. Deep Neural Networks (DNNs) are good candidates [21, 22].
- *Tracking:* pattern recognition is always a computationally challenging step. It becomes a huge challenge in the HL-LHC environment. Adequate ML techniques may provide a solution that scales linearly with LHC intensity. Several efforts in the HEP community have started to investigate ML algorithms for track pattern recognition on many-core processors.

Data Organisation, Management and Access

The scientific reach of data-intensive experiments is limited by how fast data can be accessed and digested by computational resources. Changes in computing technology and large increases in data volume require new computational models [92], compatible with budget constraints. The integration of newly emerging data analysis paradigms into our computational model has the potential to enable new analysis methods and increase scientific output. The field, as a whole, has a window in which to adapt our data access and data management schemes to ones that are more suited and optimally matched to advanced computing models and a wide range of analysis applications.

Scope and Challenges

The LHC experiments currently provision and manage about an exabyte of storage, approximately half of which is archival, and half is traditional disk storage. Other experiments that will soon start data taking have similar needs, e.g., Belle II has the same data volumes as ATLAS. The HL-LHC storage requirements per year are expected to jump by a factor close to 10, which is a growth rate faster than can be accommodated by projected technology gains. Storage will remain one of the major cost drivers for HEP computing, at a level roughly equal to the cost of the computational resources. The combination of storage and analysis computing costs may restrict scientific output and the potential physics reach of the experiments, so new techniques and algorithms are likely to be required.

In devising experiment computing models for this era many factors have to be taken into account. In particular, the increasing availability of very high-speed networks may reduce the need for CPU and data co-location. Such networks may allow for more extensive use of data access over the Wide-Area Network (WAN), which may provide failover capabilities, global and federated data namespaces, and will have an impact on data caching. Shifts in data presentation and analysis models, such as the use of event-based data streaming along with more traditional dataset-based or file-based data access, will be particularly important for optimising the utilisation of opportunistic computing cycles on HPC facilities, commercial cloud resources, and campus clusters. This can potentially resolve currently limiting factors such as job eviction.

The three main challenges for data management in the HL-LHC follow:

- The experiments will significantly increase both the data rate and the data volume. The computing systems will need to handle this with as small a cost increase as possible and within evolving storage technology limitations.
- The significantly increased computational requirements for the HL-LHC era will also place new requirements on data access. Specifically, the use of new types of computing resources (cloud, HPC) that have different dynamic availability and characteristics will require more dynamic data management and access systems.
- Applications employing new techniques, such as training for machine learning or high rate data query systems, will likely be employed to meet the computational constraints and to extend physics reach. These new applications will place new requirements on how and where data is accessed and produced. Specific applications, such as training for machine learning, may require use of specialised processor resources, such as GPUs, placing further requirements on data.

The projected event complexity of data from future HL-LHC runs with high pileup and from high resolution Liquid Argon detectors at DUNE will require advanced reconstruction algorithms and analysis tools to interpret the data. The precursors of these tools, in the form of new pattern recognition and tracking algorithms, are already proving to be drivers for the compute needs of the HEP community. The storage systems that are developed, and the data management techniques that are employed, will need to be matched to these changes in computational work, so as not to hamper potential improvements.

As with computing resources, the landscape of storage solutions is trending towards heterogeneity. The ability to leverage new storage technologies as they become available into existing data delivery models is a challenge that we must be prepared for. This also implies the need to leverage "tactical storage", i.e., storage that becomes more cost-effective as it becomes available (e.g., from a cloud provider), and have a data management and provisioning system that can exploit such resources at short notice. Volatile data sources would impact many aspects of the system: catalogues, job brokering, monitoring and alerting, accounting, the applications themselves.

On the hardware side, R&D is needed in alternative approaches to data archiving to determine the possible cost/

performance tradeoffs. Currently, tape is extensively used to hold data that cannot be economically made available online. While the data is still accessible, it comes with a high latency penalty, limiting effective data access. We suggest investigating either separate direct access-based archives (e.g., disk or optical) or new models that hierarchically overlay online direct access volumes with archive space. This is especially relevant when access latency is proportional to storage density. Either approach would need to also evaluate reliability risks and the effort needed to provide data stability. For this work, we should exchange experiences with communities that rely on large tape archives for their primary storage.

Cost reductions in the maintenance and operation of storage infrastructure can be realised through convergence of the major experiments and resource providers on shared solutions. This does not necessarily mean promoting a monoculture, as different solutions will be adapted to certain major classes of use cases, type of site, or funding environment. There will always be a judgement to make on the desirability of using a variety of specialised systems, or of abstracting the commonalities through a more limited, but common, interface. Reduced costs and improved sustainability will be further promoted by extending these concepts of convergence beyond HEP and into the other large-scale scientific endeavours that will share the infrastructure in the coming decade (e.g., the SKA and CTA experiments). Efforts must be made as early as possible, during the formative design phases of such projects, to create the necessary links.

Finally, all changes undertaken must not make the ease of access to data any worse than it is under current computing models. We must also be prepared to accept the fact that the best possible solution may require significant changes in the way data is handled and analysed. What is clear is that current practices will not scale to the needs of HL-LHC and other major HEP experiments of the coming era.

Current Practices

The original LHC computing models were based on simpler models used before distributed computing was a central part of HEP computing. This allowed for a reasonably clean separation between four different aspects of interacting with data, namely data organisation, data management, data access, and data granularity. The meaning of these terms may be summarised in what follows.

- *Data organisation* is essentially how data is structured as it is written. Most data is written in files, in ROOT format, typically with a column-wise organisation of the data. The records corresponding to these columns are compressed. The internal details of this organisation are visible only to individual software applications.
- In the past, the key challenge for data management was the transition to use distributed computing in the form of the grid. The experiments developed dedicated data transfer and placement systems, along with catalogues, to move data between computing centres. Originally, computing models were rather static: data was placed at sites, and the relevant compute jobs were sent to the right locations. Since LHC startup, this model has been made more flexible to limit non-optimal pre-placement and to take into account data popularity. In addition, applications might interact with catalogues or, at times, the workflow management system does this on behalf of the applications.
- *Data access*: historically, various protocols have been used for direct reads (rfio, dcap, xrootd, etc.) where jobs are reading data explicitly staged-in or cached by the compute resource used or the site it belongs to. A recent move has been the convergence towards xrootd as the main protocol for direct access. With direct access, applications may use alternative protocols to those used by data transfers between sites. In addition, LHC experiments have been increasingly using remote access to the data, without any stage-in operations, using the possibilities offered by protocols such as xrootd or http.
- *Data granularity*: the data is split into datasets, as defined by physics selections and use cases, consisting of a set of individual files. While individual files in datasets can be processed in parallel, the files themselves are usually processed as a whole.

Before LHC turn-on, and in the first years of the LHC, these four areas were to first order optimised independently. As LHC computing matured, interest has turned to optimisations spanning multiple areas. For example, the recent use of "Data Federations" mixes up Data Management and Access. As we will see below, some of the foreseen opportunities towards HL-LHC may require global optimisations.

Thus, in this section we take a broader view than traditional data management and consider the combination of "Data Organisation, Management and Access" (DOMA) together. We believe that this fuller picture will provide important opportunities for improving efficiency and scaleability, as we enter the many-exabyte era.

Research and Development Programme

In the following, we describe tasks that will need to be carried out to demonstrate that the increased volume and complexity of data expected over the coming decade can be stored, accessed, and analysed at an affordable cost.

- Sub-file granularity, e.g., event-based, will be studied to see whether it can be implemented efficiently, and in a scalable, cost-effective manner, for all applications making use of event selection, to see whether it offers an advantage over current file-based granularity. The following tasks should be completed by 2020:

  - Quantify the impact on performance and resource utilisation of the storage and network for the main access patterns, i.e., simulation, reconstruction, analysis.
  - Assess the impact on catalogues and data distribution.
  - Assess whether event-granularity makes sense in object stores that tend to require large chunks of data for efficiency.
  - Test for improvement in recoverability from preemption, in particular when using cloud spot resources and/or dynamic HPC resources.

- We will seek to derive benefits from data organisation and analysis technologies adopted by other big data users. A proof-of-concept that involves the following tasks needs to be established by 2020 to allow full implementations to be made in the years that follow.

  - Study the impact of column-wise, versus row-wise, organisation of data on the performance of each kind of access.
  - Investigate efficient data storage and access solutions that support the use of map-reduce or Spark-like analysis services.
  - Evaluate just-in-time decompression schemes and mappings onto hardware architectures considering the flow of data, from spinning disk to memory and application.

- Investigate the role data placement optimisations can play, such as caching, to use computing resources effectively, and the technologies that can be used for this. The following tasks should be completed by 2020:

  - Quantify the benefit of placement optimisation for reconstruction, analysis, and simulation.
  - Assess the benefit of caching for Machine Learning-based applications, in particular for the learning phase, and follow-up the evolution of technology outside HEP.

In the longer term the benefits that can be derived from using different approaches to the way HEP is currently managing its data delivery systems should be studied. Two different content delivery methods will be looked at, namely Content Delivery Networks (CDN) and Named Data Networking (NDN).

- Study how to minimise HEP infrastructure costs by exploiting varied quality of service from different storage technologies. In particular, study the role that opportunistic/tactical storage can play, as well as different archival storage solutions. A proof-of-concept should be made by 2020, with a full implementation to follow in the following years.

- Establish how to globally optimise data access latency, with respect to the efficiency of using CPU, at a sustainable cost. This involves studying the impact of concentrating data in fewer, larger locations (the "data-lake" approach), and making increased use of opportunistic compute resources located further from the data. Again, a proof-of-concept should be made by 2020, with a full implementation in the following years, if successful. This R&D will be done in common with the related actions planned as part of Facilities and Distributed Computing.

Facilities and Distributed Computing

Scope and Challenges

As outlined in "Software and computing challenges", huge resource requirements are anticipated for HL-LHC running. These need to be deployed and managed across the WLCG infrastructure, which has evolved from the original ideas on deployment before LHC data-taking started [6], to be a mature and effective infrastructure that is now exploited by LHC experiments. Currently, hardware costs are dominated by disk storage, closely followed by CPU, followed by tape and networking. Naive estimates of scaling to meet HL-LHC needs indicate that the current system would need almost an order of magnitude more resources than will be available from technology evolution alone. In addition, other initiatives such as Belle II and DUNE in particle physics, but also other science projects such as SKA, will require a comparable amount of resources on the same infrastructure. Even anticipating substantial software improvements, the major challenge in this area is to find the best configuration for facilities and computing sites that make HL-LHC computing feasible. This challenge is further complicated by substantial regional differences in funding models, meaning that any solution must be sensitive to these local considerations to be effective.

There are a number of changes that can be anticipated on the timescale of the next decade that must be taken into account. There is an increasing need to use highly heterogeneous resources, including the use of HPC infrastructures (which can often have very particular setups and policies that make their exploitation challenging); volunteer computing (which is restricted in scope and unreliable, but can be a significant resource); and cloud computing, both commercial and research. All of these offer different resource provisioning interfaces and can be significantly more dynamic than directly funded HEP computing sites. In addition, diversity of computing architectures is expected to become the norm, with different CPU architectures, as well as more specialised GPUs and FPGAs.

This increasingly dynamic environment for resources, particularly CPU, must be coupled with a highly reliable system for data storage and a suitable network infrastructure for delivering this data to where it will be processed. While CPU and disk capacity is expected to increase by respectively 15% and 25% per year for the same cost [33], the trends of research network capacity increases show a much steeper growth, such as two orders of magnitude from now to HL-LHC times [113]. Therefore, the evolution of the computing models would need to be more network centric.

In the network domain, there are new technology developments, such as Software Defined Networks (SDNs), which enable user-defined high capacity network paths to be controlled via experiment software, and which could help manage these data flows [27]. Some projects already started to explore the potential of these technologies [100] but a considerable R&D is required to prove their utility and practicality. In addition, the networks used by HEP are likely to see large increases in traffic from other science domains.

Underlying storage system technology will continue to evolve, for example towards object stores, and, as proposed in Data Organisation, Management and Access ("Data organisation, management and access"), R&D is also necessary to understand their usability and their role in the HEP infrastructures. There is also the continual challenge of assembling inhomogeneous systems and sites into an effective widely distributed worldwide data management infrastructure that is usable by experiments. This is particularly compounded by the scale increases for HL-LHC where multiple replicas of data (for redundancy and availability) will become extremely expensive.

Evolutionary change towards HL-LHC is required, as the experiments will continue to use the current system. Mapping out a path for migration then requires a fuller understanding of the costs and benefits of the proposed changes. A model is needed in which the benefits of such changes can be evaluated, taking into account hardware and human costs, as well as the impact on software and workload performance that in turn leads to physics impact. Even if HL-LHC is the use case used to build this cost and performance model, because the ten years of experience running large-scale experiments helped to define the needs, it is believed that this work, and the resulting model, will be valuable for other upcoming data intensive scientific initiatives. This includes future HEP projects, such as Belle II, DUNE and possibly ILC experiments, but also non-HEP projects, such as SKA.

Current Practices

While there are many particular exceptions, most resources incorporated into the current WLCG are done so in independently managed sites, usually with some regional organisation structure, and mostly offering both CPU and storage. The sites are usually funded directly to provide computing to WLCG, and are in some sense then "owned" by HEP, albeit often shared with others. Frequently substantial cost contributions are made indirectly, for example through funding of energy costs or additional staff effort, particularly at smaller centres. Tape is found only at CERN and at large national facilities, such as the WLCG Tier-1s [26].

Interfaces to these computing resources are defined by technical operations in WLCG. Frequently there are choices that sites can make among some limited set of approved options for interfaces. These can overlap in functionality. Some are very HEP specific and recognised as over-complex: work is in progress to get rid of them. The acceptable architectures and operating systems are also defined at the WLCG level (currently x86_64, running Scientific Linux 6 and compatible), and sites can deploy these either directly onto "bare metal" or can use an abstraction layer, such as virtual machines or containers.

There are different logical networks being used to connect sites: LHCOPN connects CERN with the Tier-1 centres and a mixture of LHCONE and generic academic networks connect other sites.

Almost every experiment layers its own customised workload and data management system on top of the base WLCG provision, with several concepts, and a few lower level components, in common. The pilot job model for workloads is ubiquitous, where a real workload is dispatched only once a job slot is secured. Data management layers aggregate files in the storage systems into datasets and manage experiment-specific metadata. In contrast to the MONARC model, sites are generally used more flexibly and homogeneously by experiments, both in workloads and in data stored.

In total, WLCG currently provides experiments with resources distributed at about 170 sites, in 42 countries, which pledge every year the amount of CPU and disk resources they are committed to delivering. The pledge process is overseen by the Computing Resource Scrutiny Group (CRSG), mandated by the funding agencies to validate the experiment requests, and to identify mismatches with site pledges. These sites are connected by 10–100 Gb links, and deliver approximately 500 k CPU cores and 1 EB of storage, of which 400 PB is disk. More than 200 M jobs are executed each day [25].

Research and Development programme

The following areas of study are ongoing, and will involve technology evaluations, prototyping, and scale tests. Several of the items below require some coordination with other topical areas discussed in this document, and some work is still needed to finalise the detailed action plan. These actions will need to be structured to meet the common milestones of informing the HL-LHC Computing Technical Design Reports (TDRs), and deploying advanced prototypes during LHC Run 3.

- Understand better the relationship between the performance and costs of the WLCG system, and how it delivers the necessary functionality to support LHC physics. This will be an ongoing process, started by the recently formed System Performance and Cost Modeling Working Group [133], and aims to provide a quantitative assessment for any proposed changes.
- Define the functionality needed to implement a federated data centre concept ("data lake") that aims to reduce the operational cost of storage for HL-LHC, and at the same time better manage network capacity, whilst maintaining the overall CPU efficiency. This would include the necessary qualities of service, and options for regionally distributed implementations, including the ability to flexibly respond to model changes in the balance between disk and tape. This work should be done in conjunction with the existing Data Organisation, Management and Access Working Group [159] to evaluate the impact of the different access patterns and data organisations envisaged.
- Building upon the experience of projects currently exploring SDN potential, define the role for this technology in managing data transfers and access and the integration strategy into experiment frameworks.
- Establish an agreement on the common data management functionality that is required by experiments, targeting a consolidation and a lower maintenance burden. The intimate relationship between the management of elements in storage systems and metadata must be recognised. This work requires coordination with the Data Processing Frameworks Working Group. It needs to address at least the following use cases:

    - processing sites that may have some small disk cache, but do not manage primary data;
    - fine-grained processing strategies that may enable processing of small chunks of data, with appropriate bookkeeping support;
    - integration of heterogeneous processing resources, such as HPCs and clouds.
- Explore scalable and uniform means of workload scheduling, which incorporate dynamic heterogenous resources, and the capabilities of finer grained processing that increases overall efficiency. The optimal scheduling of special workloads that require particular resources is clearly required.
- Contribute to the prototyping and evaluation of a quasi-interactive analysis facility that would offer a different model for physics analysis, but would also need to be integrated into the data and workload management of the experiments. This is work to be done in collaboration with groups working on new data analysis models.

Data-Flow Processing Framework

Scope and Challenges

Frameworks in HEP are used for the collaboration-wide data processing tasks of triggering, reconstruction, and simulation, as well as other tasks that subgroups of the collaboration are responsible for, such as detector alignment and calibration. Providing framework services and libraries that will satisfy the computing and data needs for future HEP experiments in the next decade, while maintaining our efficient exploitation of increasingly heterogeneous resources, is a huge challenge.

To fully exploit the potential of modern processors, HEP data processing frameworks need to allow for the parallel execution of reconstruction or simulation algorithms on multiple events simultaneously. Frameworks face the challenge of handling the massive parallelism and heterogeneity that will be present in future computing facilities, including multi-core and many-core systems, GPUs, Tensor Processing Units (TPUs), and tiered memory systems, each integrated with storage and high-speed network interconnections. Efficient running on heterogeneous resources will require a tighter integration with the computing models' higher-level systems of workflow and data management. Experiment frameworks must also successfully integrate and marshall other HEP software that may have its own parallelisation model, such as physics generators and detector simulation.

Common developments across experiments are desirable in this area, but are hampered by many decades of legacy work. Evolving our frameworks also has to be done recognising the needs of the different stakeholders in the system. This includes physicists, who are writing processing algorithms for triggering, reconstruction or analysis; production managers, who need to define processing workflows over massive datasets; and facility managers, who require their infrastructures to be used effectively. These frameworks are also constrained by security requirements, mandated by the groups and agencies in charge of it.

Current Practices

Although most frameworks used in HEP share common concepts, there are, for mainly historical reasons, a number of different implementations; some of these are shared between experiments. The Gaudi framework [18] was originally developed by LHCb, but is also used by ATLAS and various non-LHC experiments. CMS uses its own CMSSW framework [19], which was forked to provide the art framework for the Fermilab Intensity Frontier experiments [71]. Belle II uses basf2 [98]. The linear collider community developed and uses Marlin [65]. The FAIR experiments use FairROOT, closely related to ALICE's AliROOT. The FAIR experiments and ALICE are now developing a new framework, which is called O2 [30]. At the time of writing, most major frameworks support basic parallelisation, both within and across events, based on a task-based model [82][38].

Each framework has a processing model, which provides the means to execute and apportion work. Mechanisms for this are threads, tasks, processes, and inter-process communication. The different strategies used reflect different trade-offs between constraints in the programming model, efficiency of execution, and ease of adapting to inhomogeneous resources. These concerns also reflect two different behaviours: firstly, maximising throughput, where it is most important to maximise the number of events that are processed by a given resource; secondly, minimising latency, where the primary constraint is on how long it takes to calculate an answer for a particular datum.

Current practice for throughput maximising system architectures have constrained the scope of framework designs. Framework applications have largely been viewed by the system as a batch job with complex configuration, consuming resources according to rules dictated by the computing model: one process using one core on one node, operating independently with a fixed size memory space on a fixed set of files (streamed or read directly). Only recently has CMS broken this tradition starting at the beginning of Run 2, by utilising all available cores in one process space using threading. ATLAS is currently using a multi-process fork-and-copy-on-write solution to remove the constraint of one core/process. Both experiments were driven to solve this problem by the ever-growing need for more memory per process brought on by the increasing complexity of LHC events. Current practice manages systemwide (or facility-wide) scaling by dividing up datasets, generating a framework application configuration, and scheduling jobs on nodes/cores to consume all available resources. Given anticipated changes in hardware (heterogeneity, connectivity, memory, storage) available at computing facilities, the interplay between workflow and workload management systems and framework applications need to be carefully examined. It may be advantageous to permit framework applications (or systems) to span multi-node resources, allowing them to be first-class participants in the business of scaling within a facility. In our community some aspects of this approach, which maps features with microservices or function as a service, is being pioneered by the O2 framework.

Research and Development programme

By the end of 2018: review the existing technologies that are the important building blocks for data processing frameworks and reach agreement on the main architectural concepts for the next generation of frameworks. Community meetings and workshops, along the lines of the original Concurrency Forum, are envisaged to foster collaboration in this work [44]. This includes the following:

- Libraries used for concurrency, their likely evolution and the issues in integrating the models used by detector simulation and physics generators into the frameworks.
- Functional programming, as well as domain specific languages, as a way to describe the physics data processing that has to be undertaken rather than how it has to be implemented. This approach is based on the same concepts as the idea for functional approaches for (statistical) analysis as described in "Data analysis and interpretation".
- Analysis of the functional differences between the existing frameworks and the different experiment use cases.

By 2020: prototype and demonstrator projects for the agreed architectural concepts and baseline to inform the HL-LHC Computing TDRs and to demonstrate advances over what is currently deployed. The following specific items will have to be taken into account:

- These prototypes should be as common as possible between existing frameworks, or at least several of them, as a proof-of-concept of effort and component sharing between frameworks for their future evolution. Possible migration paths to more common implementations will be part of this activity.
- In addition to covering the items mentioned for the review phase, they should particularly demonstrate possible approaches for scheduling the work across heterogeneous resources and using them efficiently, with a particular focus on the efficient use of co-processors, such as GPUs.
- They need to identify data model changes that are required for an efficient use of new processor architectures (e.g., vectorisation), and for scaling I/O performance in the context of concurrency.
- Prototypes of a more advanced integration with workload management, taking advantage in particular of the

advanced features available at facilities for a finer control of the interactions with storage and network, and dealing efficiently with the specificities of HPC resources.

By 2022: production-quality framework libraries usable by several experiment frameworks, covering the main areas successfully demonstrated in the previous phase. During these activities we expect at least one major paradigm shift to take place on this 5-year time scale. It will be important to continue discussing their impact within the community, which will be ensured through appropriate cross-experiment workshops dedicated to data processing frameworks.

Conditions Data

Scope and Challenges

Conditions data is defined as the non-event data required by data-processing software to correctly simulate, digitise or reconstruct the raw detector event data. The non-event data discussed here consists mainly of detector calibration and alignment information, with some additional data describing the detector configuration, the machine parameters, as well as information from the detector control system.

Conditions data is different from event data in many respects, but one of the important differences is that its volume scales with time rather than with the luminosity. As a consequence, its growth is limited, as compared to event data: conditions data volume is expected to be at the terabyte scale and the update rate is modest (typically O(1)Hz). However, conditions data is used by event processing applications running on a very large distributed computing infrastructure, resulting in tens of thousands of jobs that may try to access the conditions data at the same time, and leading to a very significant rate of reading (typically O(10) kHz).

To successfully serve such rates, some form of caching is needed, either using services such as web proxies (CMS and ATLAS use Frontier) or by delivering the conditions data as files distributed to the jobs. For the latter approach, CVMFS is an attractive solution due to its embedded caching, and its advanced snapshotting and branching features. ALICE have made some promising tests, and started to use this approach in Run 2; Belle II already took the same approach [161], and NA62 has also decided to adopt this solution. However, one particular challenge to be overcome with the filesystem approach is to design an efficient mapping of conditions data and metadata to files to use the CVMFS caching layers efficiently.

Efficient caching is especially important to support the high-reading rates that will be necessary for ATLAS and CMS experiments starting with Run 4. For these experiments, a subset of the conditions data is linked to the luminosity, leading to an interval of granularity down to the order of a minute. Insufficient or inefficient caching may impact the efficiency of the reconstruction processing.

Another important challenge is ensuring the long-term maintainability of the conditions data storage infrastructure. Shortcomings in the initial approach used in LHC Run 1 and Run 2, leading to complex implementations, helped to identify the key requirements for an efficient and sustainable condition data handling infrastructure. There is now a consensus among experiments on these requirements [87]: ATLAS and CMS are working on a common next-generation conditions database [123]. The Belle II experiment, which is about to start its data taking, has already developed a solution based on the same concepts and architecture. One key point in this new design is to have a server mostly agnostic to the data content with most of the intelligence on the client side. This new approach should make it easier to rely on well-established open-source products (e.g., Boost) or software components developed for the processing of event data (e.g., CVMFS). With such an approach, it should be possible to leverage technologies such as REST interfaces to simplify insertion and read operations, and make them very efficient to reach the rate levels foreseen. Also, to provide a resilient service to jobs that depend on it, the client will be able to use multiple proxies or servers to access the data.

One conditions data challenge may be linked to the use of an event service, as ATLAS is doing currently, to use efficiently HPC facilities for event simulation or processing. The event service allows better use of resources that may be volatile by allocating and bookkeeping the work done, not at the job granularity, but at the event granularity. This reduces the possibility for optimising access to the conditions data at the job level, and may lead to an increased pressure on the conditions data infrastructure. This approach is still at an early stage, and more experience is needed to better appreciate the exact impact on the conditions data.

Current Practices

The data model for conditions data management is an area where the experiments have converged on something like a best common practice. The time information for the validity of the Payloads is specified with a parameter called an Interval of Validity (IOV), which can be represented by a Run number, the ID of a luminosity section or a universal timestamp. A fully qualified set of conditions data consists of a set of payloads and their associate IOVs covering the time span required by the workload. A label called a tag identifies the version of the set and the global tag is the top-level configuration of all conditions data. For a given detector subsystem and a given IOV, a global tag will resolve to one, and only one, conditions data payload. The global tag resolves to a particular system tag via the global tag map table. A system tag consists of many intervals of validity or entries in the IOV table. Finally, each entry in the IOV table maps to a payload via its unique hash key.

A relational database is a good choice for implementing this design. One advantage of this approach is that a payload has a unique identifier, its hash key, and this identifier is the only way to access it. All other information, such as tags and IOV, is metadata used to select a particular payload. This allows a clear separation of the payload data from the metadata, and may allow use of a different backend technology to store the data and the metadata. This has potentially several advantages:

- Payload objects can be cached independently of their metadata, using the appropriate technology, without the constraints linked to metadata queries.
- Conditions data metadata are typically small compared to the conditions data themselves, which makes it easy to export them as a single file using technologies such as SQLite. This may help for long-term data preservation.
- IOVs, being independent of the payload, can also be cached on their own.

A recent trend is the move to full reconstruction online, where the calibrations and alignment are computed and applied in the High Level Trigger (HLT). This is currently being tested by ALICE and LHCb, who will adopt it for use in Run 3. This will offer an opportunity to separate the distribution of conditions data to reconstruction jobs and analysis jobs, as they will not run on the same infrastructure. However, running reconstruction in the context of the HLT will put an increased pressure on the access efficiency to the conditions data, due to the HLT time budget constraints.

Research and Development Programme

R&D actions related to Conditions databases are already in progress, and all the activities described below should be completed by 2020. This will provide valuable input for the future HL-LHC TDRs, and allow these services to be deployed during Run 3 to overcome the limitations seen in today's solutions.

- File-system view of conditions data for analysis jobs: study how to leverage advanced snapshotting/branching features of CVMFS for efficiently distributing conditions data as well as ways to optimise data/metadata layout to benefit from CVMFS caching. Prototype production of the file-system view from the conditions database.
- Identify and evaluate industry technologies that could replace HEP-specific components.
- ATLAS: migrate current implementations based on COOL to the proposed REST-based approach; study how to avoid moving too much complexity on the client side, in particular for easier adoption by subsystems, e.g., possibility of common modules/libraries. ALICE is also planning to explore this approach for the future, as an alternative or to complement the current CVMFS-based implementation.

Visualisation

Scope and Challenges

In modern High Energy Physics (HEP) experiments, visualisation of data has a key role in many activities and tasks across the whole data processing chain: detector development, monitoring, event generation, reconstruction, detector simulation, data analysis, as well as outreach and education.

Event displays are the main tool to explore experimental data at the event level and to visualise the detector itself. There are two main types of application: firstly, those integrated in the experiments' frameworks, which are able to access and visualise all the experiments' data, but at a cost in terms of complexity; secondly, those designed as cross-platform applications, lightweight and fast, delivering only a simplified version or a subset of the event data. In the first case, access to data is tied intimately to an experiment's data model (for both event and geometry data) and this inhibits portability; in the second, processing the experiment data into a generic format usually loses some detail and is an extra processing step. In addition, there are various graphical backends that can be used to visualise the final product, either standalone or within a browser, and these can have a substantial impact on the types of devices supported.

Beyond event displays, HEP also uses visualisation of statistical information, typically histograms, which allow the analyst to quickly characterise the data. Unlike event displays, these visualisations are not strongly linked to the detector geometry, and often aggregate data from multiple events. Other types of visualisation are used to display non-spatial data, such as graphs for describing the logical structure of the detector or for illustrating dependencies between the data products of different reconstruction algorithms.

The main challenges in this domain are in the sustainability of the many experiment-specific visualisation tools when common projects could reduce duplication and increase quality and long-term maintenance. The ingestion of events and other data could be eased by common formats, which would need to be defined and satisfy all users. Changes to support a client–server architecture would help broaden the ability to support new devices, such as mobile phones. Making a good choice for the libraries used to render 3D shapes is also key, impacting on the range of output devices that can be supported and the level of interaction with the user. Reacting to a fast-changing technology landscape is very important—HEP's effort is limited and generic solutions can often be used with modest effort. This applies strongly to non-event visualisation, where many open source and industry standard tools can be exploited.

Current Practices

Three key features characterise almost all HEP event displays:

- *Event-based workflow*: applications access experimental data on an event-by-event basis, visualising the data collections belonging to a particular event. Data can be related to the actual physics events (e.g., physics objects such as jets or tracks) or to the experimental conditions (e.g., detector descriptions, calibrations).
- *Geometry visualisation*: The application can display the geometry of the detector, as retrieved from the experiments' software frameworks, or a simplified description, usually for the sake of speed or portability.
- *Interactivity*: applications offer different interfaces and tools to users, to interact with the visualisation itself, select event data, and set cuts on objects' properties.

Experiments have often developed multiple event displays that either take the full integration approach explained above or are standalone and rely on extracted and simplified data.

The visualisation of data can be achieved through the low level OpenGL API, by the use of higher-level OpenGL-based libraries, or within a web browser using WebGL. Using OpenGL directly is robust and avoids other dependencies, but implies a significant effort. Instead of using the API directly, a library layer on top of OpenGL (e.g., Coin3D) can more closely match the underlying data, such as geometry, and offers a higher level API that simplifies development. However, this carries the risk that if the library itself becomes deprecated, as has happened with Coin3D, the experiment needs to migrate to a different solution or to take on the maintenance burden itself. Standalone applications often use WebGL technology to render 3D objects inside a web browser. This is a very convenient way of rendering 3D graphics, due to the cross-platform nature of web technologies, and offers many portability advantages (e.g., easier support for mobile or virtual reality devices), but at some cost of not supporting the most complex visualisations requiring heavy interaction with the experiments' data.

In recent years, video game engines, such as Unity [50] or the Unreal Engine [117], have become particularly popular in the game and architectural visualisation industry. They provide very sophisticated graphics engines and offer a lot of tools for user interaction, such as menu systems or native handling of VR devices. They are well supported by industry and tend to have a long lifespan (Unreal Engine is now 20 years old and is still very popular). However, such engines are meant to be used as development frameworks and their usage in HEP code is not always evident. Code should be developed within them, while in HEP framework-based applications we often want to use graphics libraries that can be integrated in existing code. A number of HEP collaborations have started experimenting in building event display tools with such engines, among them Belle II and ATLAS, but their use is currently limited to the display of simplified data only.

The new client–server architecture proposed as one of the visualisation R&D activities will ease the usage of WebGL technologies and game engines in HEP.

For statistical data, ROOT has been the tool of choice in HEP for many years and satisfies most use cases. However, increasing use of generic tools and data formats means Matplotlib (Python) or JavaScript based solutions (used, for example, in Jupyter notebooks) have made the landscape more diverse. For visualising trees or graphs interactively, there are many generic offerings and experiments have started to take advantage of them.

Research and Development Roadmap

The main goal of R&D projects in this area will be to develop techniques and tools that let visualisation applications and event displays be less dependent on specific experiments' software frameworks, leveraging common packages and common data formats. Exporters and interface packages will be designed as bridges between the experiments' frameworks, needed to access data at a high level of detail, and the common packages based on the community standards that this group will develop.

As part of this development work, demonstrators will be designed to show the usability of our community solutions and tools. The goal will be to get a final design of those tools so that the experiments can depend on them in their future developments.

The working group will also work towards a more convenient access to geometry and event data, through a client–server interface [23]. In collaboration with the Data Access and Management Working Group, an API or a service to deliver streamed event data would be designed.

The work above should be completed by 2020.

Beyond that point, the focus will be on developing the actual community-driven tools, to be used by the experiments for their visualisation needs in production, potentially taking advantage of new data access services.

The workshops that were held as part of the CWP process (HSF Visualization Workshop, see Appendix A) were felt to be extremely useful for exchanging knowledge between developers in different experiments, fostering collaboration and in bringing in ideas from outside the community. These will now be held as an annual events and will facilitate work on the common R&D plan.

Software Development, Deployment, Validation and Verification

Scope and Challenges

Modern HEP experiments are often large distributed collaborations with several hundred people actively writing software. It is, therefore, vital that the processes and tools used for development are streamlined to ease the process of contributing code and to facilitate collaboration between geographically separated peers. At the same time, we must properly manage the whole project, ensuring code quality, reproducibility, and maintainability with the least effort possible. Making sure this happens is largely a continuous process and shares a lot with non-HEP specific software industries.

Work is ongoing to track and promote solutions in the following areas:

- Distributed development of software components, including the tools and processes required to do so (code organisation, documentation, issue tracking, artefact building), and the best practices in terms of code and people management.
- Software quality, including aspects such as modularity and reusability of the developed components, architectural and performance best practices.
- Software sustainability, including both development and maintenance efforts, as well as best practices given long timescales of HEP experiments.
- Deployment of software and interaction with operations teams.
- Validation of the software both at small scales (e.g., best practices on how to write a unit test) and larger ones (large-scale validation of data produced by an experiment).
- Software licensing and distribution, including their impact on software interoperability.
- Recognition of the significant contribution that software makes to HEP as a field (also see “Training and careers” regarding career recognition).

HEP-specific challenges derive from the fact that HEP is a large, inhomogeneous community with multiple sources of funding, mostly formed of people belonging to university groups and HEP-focused laboratories. Software development effort within an experiment usually encompasses a huge range of experience and skills, from a few more or less full-time experts to many physicist programmers with little formal software training. In addition, the community is split between different experiments that often diverge in timescales, size, and resources. Experiment software is usually divided in two separate use cases: production (being it data acquisition, data reconstruction or simulation) and user analysis, whose requirements and lifecycles are completely different. The former is very carefully managed in a centralised and slow-moving manner, following the schedule of the experiment itself. The latter is much more dynamic and strongly coupled with conferences or article publication timelines. Finding solutions that adapt well to both cases is not always obvious or even possible.

Current Practices

Due to significant variations between experiments at various stages of their lifecycles, there is a huge variation in practice across the community. Thus, here we describe best practice, with the understanding that this ideal may be far from the reality for some developers.

It is important that developers can focus on the design and implementation of the code and do not have to spend a lot of time on technical issues. Clear procedures and policies must exist to perform administrative tasks in an easy and quick way. This starts with the setup of the development environment. Supporting different platforms not only allows developers to use their machines directly for development, it also provides a check of code portability. Clear guidance and support for good design must be available in advance of actual coding.

To maximise productivity, it is very beneficial to use development tools that are not HEP-specific. There are many open source projects that are of similar scale to large experiment software stacks and standard tools are usually well documented. For source control HEP has generally chosen to move to *git* [66], which is very welcome, as it also brings an alignment with many open source projects and commercial organisations. A major benefit that has come with this technical choice is the use of social coding sites, such as *GitHub* [67] and *GitLab* [68], where code sharing and code review are far superior compared to previous solutions. Likewise, *CMake* [39] is widely used for the builds of software packages, both within HEP and outside. Packaging many build products together into a software stack is an area that still requires close attention with respect to active developments (the HSF has an active working group here).

Proper testing of changes to code should always be done in advance of a change request to be accepted. Continuous integration, where ‘merge’ or ‘pull’ requests are built and tested in advance, is now standard practice in the open source community and in industry. Continuous integration can run unit and integration tests, and can also incorporate code quality checks and policy checks that help improve the consistency and quality of the code at low human cost.

Further validation on different platforms and at large scales must be as automated as possible, including the deployment of build artefacts for production.

Training ("Training and careers") and documentation are key to efficient use of developer effort. Documentation must cover best practices and conventions as well as technical issues. For documentation that has to be specific, the best solutions have a low barrier of entry for new contributors, but also allow and encourage review of material. Consequently, it is very useful to host documentation sources in a repository with a similar workflow to code, and to use an engine that translates the sources into modern web pages.

Recognition of software work as a key part of science has resulted in a number of journals where developers can publish their work [132]. Journal publication also disseminates information to the wider community in a permanent way and is the most established mechanism for academic recognition. Publication in such journals provides proper peer review, beyond that provided in conference papers, so it is valuable for recognition as well as dissemination. However, this practice is not widespread enough in the community and needs further encouragement.

Research and Development Programme

HEP must endeavour to be as responsive as possible to developments outside of our field. In terms of hardware and software tools, there remains great uncertainty as to what the platforms offering the best value for money will be on the timescale of a decade. It therefore behoves us to be as generic as possible in our technology choices, retaining the necessary agility to adapt to this uncertain future.

Our vision is characterised by HEP being current with technologies and paradigms that are dominant in the wider software development community, especially for open-source software, which we believe to be the right model for our community. To achieve that aim, we propose that the community establishes a development forum that allows for technology tracking and discussion of new opportunities. The HSF can play a key role in marshalling this group and in ensuring its findings are widely disseminated. In addition, having wider and more accessible training for developers in the field, that will teach the core skills needed for effective software development, would be of great benefit.

Given our agile focus, it is better to propose here projects and objectives to be investigated in the short to medium term, alongside establishing the means to continually review and refocus the community on the most promising areas. The main idea is to investigate new tools as demonstrator projects where clear metrics for success in a reasonable time should be established to avoid wasting community effort on initially promising products that fail to live up to expectations.

Ongoing activities and short-term projects, to complete by 2020, include the following:

- Establish a common forum for the discussion of HEP software problems. This should be modeled along the lines of the Concurrency Forum [44], which was very successful in establishing demonstrators and prototypes that were used as experiments started to develop parallel data processing frameworks.
- Continue the HSF working group on Packaging, with more prototype implementations based on the strongest candidates identified so far.
- Provide practical advice on how to best set up new software packages, developing on the current project template work, and working to advertise this within the community.
- Work with HEP experiments and other training projects to provide accessible core skills training to the community (see "Training and careers"). This training should be experiment-neutral, but could be usefully combined with the current experiment specific training. Specifically, this work can build on, and collaborate with, recent highly successful initiatives such as the LHCb *Starterkit* [89] and ALICE *Juniors* [20], and with established generic training initiatives such as *Software Carpentry* [125].
- Strengthen links with software communities and conferences outside of the HEP domain, presenting papers on the HEP experience and problem domain. The Scientific Computing with Python (SciPy), the Supercomputing Conferences (SCxx), the Conference of Research Software Engineers *(RSE)*, and the Workshops on Sustainable Software for Science: Practice and Experiences (WSSSPE) would all be useful meetings to consider.
- Write a paper that looks at case studies of successful and unsuccessful HEP software developments and that draws specific conclusions and advice for future projects.
- Strengthen the publication record for important HEP software packages. Both peer-reviewed journals [132] and citable software version records (such as DOIs obtained via Zenodo [164]).

Longer term projects, to conclude by 2022, include the following:

- Prototype C++ refactoring tools, with specific use cases in migrating HEP code.
- Prototyping of portable solutions for exploiting modern vector hardware on heterogenous platforms.
- Support the adoption of industry standards and solutions over HEP-specific implementations whenever possible.
- Develop tooling and instrumentation to measure software performance where tools with sufficient capabilities are not available from industry, especially in the domain of

concurrency. This should primarily aim to further developments of existing tools, such as *igprof* [58], rather than to develop new ones.
- Develop a common infrastructure to gather and analyse data about experiments' software, including profiling information and code metrics, and to ease sharing across different user communities.
- Undertake a feasibility study of a common toolkit for statistical analysis that would be of use in regression testing for experiment's simulation and reconstruction software.

Data and Software Preservation

Scope and Challenges

Given the very large investment in particle physics experiments, it is incumbent upon physicists to preserve the data and the knowledge that leads to scientific results in a manner such that this investment is not lost to future generations of scientists. For preserving "data", at whatever stage of production, many of the aspects of the low level bit-wise preservation have been covered by the Data Preservation for HEP group [52]. "Knowledge" preservation encompasses the more challenging aspects of retaining processing and analysis software, documentation, and other components necessary for reusing a given dataset. Preservation of this type can enable new analyses on older data, as well as a way to revisit the details of a result after publication. The latter can be especially important in resolving conflicts between published results, applying new theoretical assumptions, evaluating different theoretical models, or tuning new modeling techniques.

Preservation enabling reuse can offer tangible benefits within a given experiment. The preservation of software and workflows such that they can be shared enhances collaborative work between analysts and analysis groups, providing a way of capturing the knowledge behind a given analysis during the review process. It enables easy transfer of knowledge to new students or analysis teams, and could establish a manner by which results can be generated automatically for submission to central repositories, such as HEPData [93]. Preservation within an experiment can provide ways of reprocessing and reanalysing data that could have been collected more than a decade earlier. Benefits from preservation are derived internally whether or not analysis work is approved through the publication approval process for an experiment. Providing such immediate benefits makes the adoption of data preservation in experiment workflows particularly desirable.

A final series of motivations comes from the potential re-use by others outside of the HEP experimental community. Significant outreach efforts to bring the excitement of analysis and discovery to younger students have been enabled by the preservation of experimental data and software in an accessible format. Many examples also exist of phenomenology papers reinterpreting the results of a particular analysis in a new context. This has been extended further with published results based on the reanalysis of processed data by scientists outside of the collaborations. Engagement of external communities, such as machine learning specialists, can be enhanced by providing the capability to process and understand low-level HEP data in portable and relatively platform-independent way, as happened with the Kaggle ML challenges [5]. This allows external users direct access to the same tools and data as the experimentalists working in the collaborations. Connections with industrial partners, such as those fostered by CERN OpenLab, can be facilitated in a similar manner.

Preserving the knowledge of analysis, given the extremely wide scope of how analysts do their work and experiments manage their workflows, is far from easy. The level of reuse that is applicable needs to be identified, and so a variety of preservation systems will probably be appropriate given the different preservation needs between large central experiment workflows and the work of an individual analyst. The larger question is to what extent common low-level tools can be provided that address similar needs across a wide scale of preservation problems. These would range from capture tools, that preserve the details of an analysis and its requirements, to ensuring that software and services needed for a workflow would continue to function as required.

The above-mentioned steps are consistent with the FAIR data principles that are increasingly being mandated by funding agencies [140].

Current Practices

Each of the LHC experiments has adopted a data access and/or data preservation policy, all of which can be found on the CERN Open Data Portal [34]. All of the LHC experiments support public access to some subset of the data in a highly reduced data format for the purposes of outreach and education. CMS has gone one step further, releasing substantial datasets in an Analysis Object Data (AOD) format that can be used for new analyses. The current data release includes simulated data, virtual machines that can instantiate the added analysis examples, and extensive documentation [40]. ALICE has promised to release 10% of their processed data after a five-year embargo and has released 2010 data at this time [10]. LHCb is willing to make access to reconstructed data available, but is unable to commit to a specific timescale due to resource limitations. A release of ntuple-level data for one high profile analysis, aimed primarily at educational activities, is currently in preparation. ATLAS has chosen a different direction for data release: data associated with journal publications is made available, and ATLAS also strives to make available additional material that allows reuse and reinterpretations of the data in the context of new theoretical models [13]. ATLAS is exploring how to provide the capability for reinterpretation of searches in the future via a service such as RECAST [49], in which the original internal analysis code (including full detector simulation and reconstruction) is preserved, as opposed to the re-coding approach with object-efficiency calibrations used by external reinterpretation toolkits. All experiments frequently provide detailed supplemental data along with publications to allow for more detailed comparisons between results, or even reinterpretation.

The LHC experiments have not yet set a formal policy addressing the new capabilities of the CERN Analysis Preservation Portal (CAP) [32] and whether or not some use of it will be required or merely encouraged. All of them support some mechanisms for internal preservation of the knowledge surrounding a physics publication [53].

Research and Development Programme

There is a significant programme of work already happening in the data preservation area. The feasibility and cost of common base services have been studied for bit preservation, the preservation of executable software environments, and the structured capturing of analysis metadata [122].

The goals presented here should be orchestrated in conjunction with projects conducted by the R&D programmes of other working groups, since the questions addressed are common. Goals to address on the timescale of 2020 are:

- Include embedded elements for the capture of preservation information and metadata and tools for the archiving of this information in developing a prototype analysis ecosystem(s). This should include an early demonstration of the CAP analysis preservation portal with a working UI.
- Demonstrate the capability to provision and execute production workflows for experiments that are composed of multiple independent containers.
- Collection of analysis use cases and elements that are necessary to preserve to enable re-use and to ensure these analyses can be captured in developing systems. This should track analysis evolution towards possible Big Data environments and determine any elements that are difficult to capture, spawning further R&D.
- Evaluate, in the preservation area, the full potential and limitations of sandbox and “freezing” technologies, possibly coupled with version and history control software distribution systems.
- Develop prototypes for the preservation and validation of large-scale production executables and workflows.
- Integrate preservation capabilities into newly developed computing tools and workflows.
- Extension and standardisation of the final data and analysis preservation scheme via HEPData, Rivet and/or other reinterpretation tools. This could be used to preserve a sufficiently detailed re-usable record of many LHC Run 2 research outputs.

This would then lead naturally to deployed solutions that support data preservation in the 2020–2022 time frame for the HEP experimental programmes, in particular an analysis ecosystem that enables reuse for any analysis that can be conducted in the ecosystem, and a system for the preservation and validation of large-scale production workflows.

Security

Scope and Challenges

Security is a cross-cutting area that impacts our projects, collaborative work, users, and software infrastructure fundamentally. It crucially shapes our reputation, our collaboration, the trust between participants, and the users’ perception of the quality and ease of use of our services.

There are three key areas:

- Trust and policies; this includes trust models, policies, compliance, data protection issues.
- Operational security; this includes threat intelligence, security operations, incident response.
- Authentication and authorisation; this includes identity management, identity federation, access control.

The evolution in the security domain requires the HEP community to work in collaboration with the various national security organisations and policy groups, building on many relationships that are already established.

Trust and policies Data Protection defines the boundaries that enable HEP work to be conducted, in particular regarding data sharing aspects, for example between the EU and the US. It is essential to establish a trusted personal data exchange framework, minimising the amount of personal data to be processed and ensuring legal compliance.

Beyond legal compliance and best practice, offering open access to scientific resources and achieving shared goals requires prioritising the protection of people and science, including the mitigation of the effects of surveillance programs on scientific collaborations.

On the technical side, it is necessary to adapt the current, aging trust model and security architecture relying solely on X.509 (which is no longer the direction industry is taking), to include modern data exchange design, for example involving commercial providers or hybrid clouds. The future of our infrastructure involves increasingly diverse resource providers connected through cloud gateways. For example, HEPCloud [62] at FNAL aims to connect Amazon, Google Clouds, and HPC centres with our traditional grid computing resources. The HNSciCloud European Project [142] aims to support the enhancement of commercial cloud providers to be leveraged by the scientific community. These are just two out of a number of endeavours. As part of this modernisation, a transition is needed from a model in which all participating organisations are bound by custom HEP security policies to a more flexible approach where some partners are not in a position to adopt such policies.

Operational security and threat intelligence As attacks have become extremely sophisticated and costly to defend against, the only cost-effective strategy is to address security threats together, as a community. This involves constantly striving to liaise with external organisations, including security vendors and law enforcement entities, to enable the sharing of indicators of compromise and threat intelligence between all actors. For organisations from all sectors, including private companies, governments, and academia, threat intelligence has become the main means by which to detect and manage security breaches.

In addition, a global forum for HEP and the larger Research and Education (R&E) community needs to be built, where security experts feel confident enough to share threat intelligence and security expertise. A key to success is to ensure a closer collaboration between HEP security contacts and campus security. The current gap at many HEP organisations is both undermining the community's security posture and reducing the effectiveness of the HEP security strategy.

There are several very active trust groups in the HEP community where HEP participants share threat intelligence and organise coordinated incident response [59, 111, 139]. There is unfortunately still no global Research and Education forum for incident response, operational security, and threat intelligence sharing. With its mature security operations and dense, global network of HEP organisations, both of which are quite unique in the research sector, the HEP community is ideally positioned to contribute to such a forum and to benefit from the resulting threat intelligence, as it has exposure, sufficient expertise, and connections to lead such an initiative. It may play a key role in protecting multiple scientific domains at a very limited cost.

There will be many technology evolutions as we start to take a serious look at the next-generation internet. For example, IPv6 is one upcoming change that has yet to be fully understood from the security perspective. Another high impact area is the Internet of Things (IoT), connected devices on our networks that create new vectors of attack.

It will become necessary to evaluate and maintain operational security in connected environments spanning public, private, and hybrid clouds. The trust relationship between our community and such providers has yet to be determined, including the allocation of responsibility for coordinating and performing vulnerability management and incident response. Incompatibilities between the e-Infrastructure approach to community-based incident response and the "pay-for-what-you-break" model of certain commercial companies may come to light and must be resolved.

Authentication and authorisation infrastructure It is now largely acknowledged that end-user certificates are challenging to manage and create a certain entrance barrier to our infrastructure for early career researchers. Integrating our access control management system with new, user-friendly technologies and removing our dependency on X.509 certificates is a key area of interest for the HEP Community.

An initial step is to identify other technologies that can satisfy traceability, isolation, privilege management and other requirements necessary for HEP workflows. The chosen solution should prioritise limiting the amount of change required to our services and follow accepted standards to ease integration with external entities, such as commercial clouds and HPC centres.

Trust federations and inter-federations, such as the R&E standard eduGAIN [54], provide a needed functionality for Authentication. They can remove the burden of identity provisioning from our community and allow users to leverage their home organisation credentials to access distributed computing resources. Although certain web-based services have enabled authentication via such federations, uptake is not yet widespread. The challenge remains to have the necessary attributes published by each federation to provide robust authentication.

The existing technologies leveraged by identity federations, e.g., the Security Assertion Markup Language (SAML), have not supported non-web applications historically. There is momentum within the wider community to develop next-generation identity federations [103] that natively support a wider range of clients. In the meantime, there are several viable interim solutions that are able to provision users with the token required to access a service (such as X.509) transparently, translated from their home organisation identity.

Although non-X509 federated identity provides a potential solution for our challenges in Authentication, authorisation should continue to be tightly controlled by the HEP community. Enabling Virtual Organisation (VO) membership for federated credentials and integrating such a workflow with existing identity vetting processes is a major topic currently being worked on, in particular within the WLCG community. Commercial clouds and HPC centres have fundamentally different access control models and technologies from our grid environment. We shall need to enhance our access control model to ensure compatibility and translate our grid-based identity attributes into those consumable by such services.

Current Activities

Multiple groups are working on policies and establishing a common trust framework, including the EGI Security Policy Group [55] and the Security for Collaboration among Infrastructures working group [119].

Operational security for the HEP community is being followed up in the WLCG Working Group on Security Operations Centres [160]. The HEP Community is actively involved in multiple operational security groups and trust groups, facilitating the exchange of threat intelligence and incident response communication. WISE [158] provides a forum for e-Infrastructures to share and develop security best practices and offers the opportunity to build relationships between security representatives at multiple e-infrastructures of interest to the HEP community.

The evolution of Authentication and Authorisation is being evaluated in the recently created WLCG Working Group on Authorisation. In parallel, HEP is contributing to a wider effort to document requirements for multiple Research Communities through the work of FIM4R [60]. Participation of CERN and a few other major WLCG sites in the European Authentication and Authorisation for Research and Collaboration (AARC) project [16] provides the opportunity to ensure that any directions chosen are consistent with those taken by the wider community of research collaborations. The flow of attributes between federated entities continues to be problematic, disrupting the authentication flow. Trust between service providers and identity providers is still evolving, and efforts within the R&E Federations Group (REFEDS) [151] and the AARC project aim to address the visibility of both the level of assurance of identities and the security capability of federation participants (through Sirtfi [154]).

Research and Development Programme

Over the next decade, it is expected that considerable changes will be made to address security in the domains highlighted above. The individual groups, in particular those mentioned above, working in the areas of trust and policies, operational security, authentication and authorisation, and technology evolutions, are driving the R&D activities. These groups are generally much broader than just the HEP community. The list below summarises the most important actions:

Trust and policies

- By 2020:
  - Define and adopt policies in line with new EU Data Protection requirements.
  - Develop frameworks to ensure trustworthy interoperability of infrastructures and communities.
- By 2022:
  - Create and promote community driven incident response policies and procedures.

Operational security and threat intelligence

- By 2020:
  - Offer a reference implementation, or at least specific guidance, for a Security Operation Centre deployment at HEP sites, enabling them to take action based on threat intelligence shared within the HEP community.
- By 2022:
  - Participate in the founding of a global Research and Education Forum for incident response, since responding as a global community is the only effective solution against global security threats.
  - Build the capabilities to accommodate more participating organisations and streamline communication workflows, within and outside HEP, including maintaining a list of security contacts, secure communications channels, and security incident response mechanisms.
  - Reinforce the integration of HEP security capabilities with their respective home organisation, to ensure adequate integration of HEP security teams and site security teams.
- By 2025:
  - Prepare adequately as a community, to enable HEP organisations to operate defendable services against more sophisticated threats, stemming both from global cyber-criminal gangs targeting HEP resources (finance systems, intellectual property, ransomware), as well as from state actors targeting the energy and research sectors with advanced malware.

Authentication and authorisation

- By 2020:
  - Ensure that ongoing efforts in trust frameworks are sufficient to raise the level of confidence in non-X509 federated identities to the equivalent of X.509, at which stage they could be a viable alternative to both grid certificates and CERN accounts.
  - Participate in setting directions for the future of identity federations, through the FIM4R [60] community.
- By 2022:
  - Overhaul the current Authentication and Authorisation infrastructure, including Token Translation, integration with Community IdP-SP Proxies, and Membership Management tools. Enhancements in this area are needed to support a wider range of user identities for WLCG services.

Training and Careers

For HEP computing to be as successful as possible, the careers and skills of the individuals who participate must be considered. Ensuring that software developers can acquire the necessary skills and obtain successful careers is considered an essential goal of the HSF, which has the following specific objectives in its mission:

- To provide training opportunities for developers; this should include the support to the software schools for young scientists and computer engineers, and of a permanent training infrastructure for accomplished developers;
- To provide career support for developers, for instance by listing job opportunities and by helping to shape well-defined career paths that provide advancement opportunities on a par with those in, for example, detector construction;
- To increase the visibility of the value of software developers in HEP, recognising that it has scientific research value on an equal footing with other activities, and acknowledging and advocating for researchers who choose this as their speciality.

Training Challenges

HEP is facing major challenges with its software and computing that require innovative solutions based on the proper adoption of new technologies. More and more technologies are emerging as scientific communities and industry face similar challenges and produce solutions relevant to us. Integrating such technologies in our software and computing infrastructure requires specialists, but it is also important that a large fraction of the community is able to use these new tools and paradigms. Specific solutions and optimisations must be implemented by the HEP community itself, since many advanced requirements are unique to our field.

There is a very close collaboration, even overlap, in HEP between users of software and developers. This has given experiments an agility that was often essential for success in the past. Many details of experiment data cannot be known before data taking has started, and each change in detector technology or machine performance improvement can have important consequences for the software and computing infrastructure. In the case of detectors, engineers and physicists are required to have a good understanding of each other's field of expertise. In the same way, it is necessary that physicists understand some of the complexities of writing software, and that software experts are able to fathom the requirements of physics problems.

Training must address an audience with very diverse computing skills, ranging from novice programmers to advanced developers and users. It must be used to spread best software engineering practices and software technologies to a very large number of people, including the physicists involved across the whole spectrum of data processing tasks, from triggering to analysis. It must be done by people who have a sound knowledge of the scientific and technical details, who prepare training material despite the many calls on their time. Training thus needs proper recognition to ensure that it happens and is carried out well.

HEP is seen as an interesting, innovative, and challenging field. This is a great advantage in attracting talented young people looking for experience in a challenging and diverse environment in which they can acquire skills that will be valuable, even in other fields. As discussed in Software Development ("Software development, deployment, validation and verification"), using industry standard tools across different experiments, and training people in how to use them properly, helps with people's later career prospects and makes our field even more attractive. At the same time, experiments have a scientific programme to accomplish and also to focus on the specific training required to accomplish their specific goals. The right balance must be found between these two requirements. It is necessary to find the right incentives to favour training activities that bring more benefits in the medium to long term, for the experiment, the community, and the careers of the trainees.

Possible Directions for Training

To increase training activities in the community, whilst taking into account the constraints of both the attendees and the trainers, we should explore new approaches to training. The current "school" model is well established, as exemplified by three well-known successful schools, the CERN School of Computing [35], the Bertinoro School of Computing [78] and the GridKa School of Computing [72]. They require a significant amount of dedicated time of all the participants, at the same time and location, and therefore, are difficult to scale to meet the needs of a large number of students. In view of this, we should identify opportunities to work with HEP experiments and other training projects to provide accessible core skills training to the community by basing them at laboratories where students can easily travel. A number of highly successful experiment-specific examples exist, such as the LHCb StarterKit [89] and ALICE Juniors [20], as well as established generic training initiatives, such as Software Carpentry [125]. As with hands-on tutorials organised during conferences and workshops, the resulting networking is an important and distinctive benefit of these events, where people build relationships with other colleagues and experts.

In recent years, several R&D projects, such as DIANA-HEP [137] and AMVA4NewPhysics [7], have had training as one of their core activities. This has provided an incentive to organise training events and has resulted in the spread of expertise on advanced topics. We believe that training should become an integral part of future major R&D projects.

New pedagogical methods, such as active training and peer training, that are complementary to schools or topical tutorials, also deserve more attention. Online material can be shared by a student and a teacher to provide the exchange of real examples and practical exercises. For example, notebook technologies, such as Jupyter, support embedding of runnable code and comments into the same document. The initial material can be easily enriched by allowing other students and experts to add comments and more examples in a collaborative way. The HSF started to experiment with this approach with WikiToLearn [157], a platform developed in Italy outside HEP that promotes this kind of training and collaborative enrichment of the training material. Projects such as ROOT have also started to provide some training material based on notebooks.

A lot of initiatives have been undertaken by the software community that HEP can benefit from, and materials have been made available in the form of online tutorials, active training, and Massive Open Online Courses (MOOCs). Some effort needs to be invested to evaluate existing courses and build a repository of selected ones that are appropriate to HEP needs. This is not a negligible task and would require some dedicated effort to reach the appropriate level of support. It should help to increase training efficiency by making it easier to identify appropriate courses or initiatives.

A model that emerged in recent years as a very valuable means of sharing expertise is to use Question and Answer (Q&A) systems, such as Stack Overflow [129]. A few such systems are run by experiments for their own needs, but this is not necessarily optimal, as the value of these services is increased by a large number of contributors with diverse backgrounds. Running a cross-experiment Q&A system has been discussed, but it has not yet been possible to converge on a viable approach, both technically and because of the effort required to run and support such a service.

Career Support and Recognition

Computer specialists in HEP are often physicists who have chosen to specialise in computing. This has always been the case and needs to continue. Nevertheless, for young people in particular, this leads to a career recognition problem, as software and computing activities are not well-recognised roles in various institutions supporting HEP research and recruiting people working in the field. The exact situation is highly dependent on policies and boundary conditions of the organisation or country, but recognition of physicists tends to be based generally on participation in data analysis or hardware developments. This is even a bigger problem if the person is spending time contributing to training efforts. This negatively impacts the future of these people and reduces the possibility of HEP engaging them in the training effort of the community when the community actually needs more people to participate in this activity. Recognition of training efforts, either by direct participation in training activities or by providing materials, is an important issue to address, complementary to the incentives mentioned above.

There is no easy solution to this problem. Part of the difficulty is that organisations, and in particular the people inside them in charge of the candidate selections for new positions and promotions, need to adapt their expectations to these needs and to the importance of having computing experts with a strong physics background as permanent members of the community. Experts writing properly engineered and optimised software can significantly reduce resource consumption and increase physics reach, which provides huge financial value to modern HEP experiments. The actual path for improvements in career recognition, as the possible incentives for participating in the training efforts, depends on the local conditions.

Conclusions

Future challenges for high energy physics in the domain of software and computing are not simply an extrapolation of the challenges faced today. The needs of the HEP programme in the high luminosity era far exceed those that can be met by simply making incremental changes to today's code and scaling up computing facilities within the anticipated budget. At the same time, the limitation in single core CPU performance is making the landscape of computing hardware far more diverse and challenging to exploit, whilst offering huge performance boosts for suitable code. Exploiting parallelism and other new techniques, such as modern machine learning, offer great promise, but will require substantial work from the community to adapt to our problems. If there were any lingering notion that software or computing could be done cheaply by a few junior people for modern experimental programmes, it should now be thoroughly dispelled.

We believe HEP software and computing requires a step change in its profile and effort to match the challenges ahead. We need investment in people who can understand the problems we face, the solutions employed today, and have the correct skills to provide innovative solutions for the future. There needs to be recognition from the whole community for the work done in this area, with a recognised career path for these experts. In addition, we will need to invest heavily in training for the whole software community as the contributions of the bulk of non-expert physicists are also vital for our success.

We know that in any future scenario development effort will be constrained, so it is vital that successful R&D projects provide sustainable software for the future. It is important to emphasise that the goal is to support the HEP physics programme in a cost effective manner, so the deployment consequences of a particular technology choice or direction must be understood with partners in distributed computing. In many areas it is recognised that different experiments could have adopted common solutions, reducing overall development effort and increasing robustness and functionality. That model of duplicated development is not sustainable. We must endeavour to achieve better coherence within HEP for future developments to build advanced, open-source projects that can be shared and supported in common. The HSF has already established itself as a forum that can facilitate this. Establishing links outside of HEP, to other academic disciplines, to industry, and to the computer science community, can strengthen both the research and production phases of new solutions. We should ensure that the best products are chosen, from inside and outside HEP, and that they receive support from all parties, aiming at technical excellence and economy of scale.

We have presented programmes of work that the community has identified as being part of the roadmap for the future. While there is always some scope to reorient current effort in the field, we would highlight the following work programmes as being of the highest priority for investment to address the goals that were set in the introduction.

Improvements in software efficiency, scalability and performance

> The bulk of CPU cycles consumed by experiments relate to the fundamental challenges of simulation and reconstruction. Thus, the work programmes in these areas, together with the frameworks that support them, are of critical importance. The sheer volumes of data involved make research into appropriate data formats and event content to reduce storage requirements vital. Optimisation of our distributed computing systems, including data and workload management, is paramount.

Enable new approaches that can radically extend physics reach

> New techniques in simulation and reconstruction will be vital here. Physics analysis is an area where new ideas can be particularly fruitful. Exploring the full potential of machine learning is one common theme that underpins many new approaches and the community should endeavour to share knowledge widely across subdomains. New data analysis paradigms coming from the Big Data industry, based on innovative parallelised data processing on large computing farms, could transform data analysis.

Ensure the long-term sustainability of the software

> Applying modern software development techniques to our codes has increased, and will continue to increase, developer productivity and code quality. There is ample scope for more common tools and common training to equip the community with the correct skills. Data Preservation makes sustainability an immediate goal of development and analysis and helps to reap the benefits of our experiments for decades to come. Support for common software used across the community needs to be recognised and accepted as a common task, borne by labs, institutes, experiments, and funding agencies.

The R&D actions proposed in this Roadmap have taken into account the charges that were laid down. When considering a specific project proposal addressing our computing challenges, that project's impact, measured against the charges, should be evaluated. Over the next decade, there will almost certainly be disruptive changes that cannot be planned for, and we must remain agile enough to adapt to these.

The HEP community has many natural subdivisions, between different regional funding agencies, between universities and laboratories, and between different experiments. It was in an attempt to overcome these obstacles, and to encourage the community to work together in an efficient and effective way, that the HEP Software Foundation was established in 2014. This Community White Paper process has been possible only because of the success of that effort in bringing the community together. The need for more common developments in the future, as underlined here, reinforces the importance of the HSF as a common point of contact between all the parties involved, strengthening our community spirit and continuing to help share expertise and identify priorities. Even though this evolution will also require projects and experiments to define clear priorities about these common developments, we believe that the HSF, as a community effort, must be strongly supported as part of our roadmap to success.

Appendix A: List of Workshops

HEP Software Foundation Workshop

Date: 23–26 Jan, 2017

Location: UCSD/SDSC (La Jolla, CA, USA)

URL: http://indico.cern.ch/event/570249/

Description: This HSF workshop at SDSC/UCSD was the first workshop supporting the CWP process. There were plenary sessions covering topics of general interest as well as parallel sessions for the many topical working groups in progress for the CWP.

Software Triggers and Event Reconstruction WG meeting

Date: 9 Mar, 2017

Location: LAL-Orsay (Orsay, France)

URL: https://indico.cern.ch/event/614111/

Description: This was a meeting of the Software Triggers and Event Reconstruction CWP working group. It was held as a parallel session at the "Connecting the Dots" workshop, which focuses on forward-looking pattern recognition and machine learning algorithms for use in HEP.

IML Topical Machine Learning Workshop

Date: 20–22 Mar, 2017

Location: CERN (Geneva, Switzerland)

*URL:*https://indico.cern.ch/event/595059

Description: This was a meeting of the Machine Learning CWP working group. It was held as a parallel session at the "Inter-experimental Machine Learning (IML)" workshop, an organisation formed in 2016 to facilitate communication regarding R&D on ML applications in the LHC experiments.

Community White Paper Follow-up at FNAL

Date: 23 Mar, 2017

Location: FNAL (Batavia, IL, USA)

*URL:*https://indico.fnal.gov/conferenceDisplay.py?confId=14032

Description: This one-day workshop was organised to engage with the experimental HEP community involved in computing and software for Intensity Frontier experiments at FNAL. Plans for the CWP were described, with discussion about commonalities between the HL-LHC challenges and the challenges of the FNAL neutrino and muon experiments

CWP Visualisation Workshop

Date: 28–30 Mar, 2017

Location: CERN (Geneva, Switzerland)

*URL:*https://indico.cern.ch/event/617054/

Description: This workshop was organised by the Visualisation CWP working group. It explored the current landscape of HEP visualisation tools as well as visions for how these could evolve. There was participation both from HEP developers and industry.

DS@HEP 2017 (Data Science in High Energy Physics)

Date: 8–12 May, 2017

Location: FNAL (Batava, IL, USA)

*URL:*https://indico.fnal.gov/conferenceDisplay.py?confId=13497

Description: This was a meeting of the Machine Learning CWP working group. It was held as a parallel session at the "Data Science in High Energy Physics (DS@HEP)" workshop, a workshop series begun in 2015 to facilitate communication regarding R&D on ML applications in HEP.

HEP Analysis Ecosystem Retreat

Date: 22–24 May, 2017

Location: Amsterdam, the Netherlands

*URL:*http://indico.cern.ch/event/613842/

*Summary report:*http://cern.ch/go/mT8w

Description: This was a general workshop, organised about the HSF, about the ecosystem of analysis tools used in HEP and the ROOT software framework. The workshop focused both on the current status and the 5–10 year time scale covered by the CWP.

CWP Event Processing Frameworks Workshop

Date: 5–6 Jun, 2017

Location: FNAL (Batavia, IL, USA)

*URL:*https://indico.fnal.gov/conferenceDisplay.py?confId=14186

Description: This was a workshop held by the Event Processing Frameworks CWP working group focused on writing an initial draft of the framework white paper. Representatives from most of the current practice frameworks participated.

HEP Software Foundation Workshop

Date: 26–30 Jun, 2017

Location: LAPP (Annecy, France)

*URL:*https://indico.cern.ch/event/613093/

Description: This was the final general workshop for the CWP process. The CWP working groups came together to present their status and plans, and develop consensus on the organisation and context for the community roadmap. Plans were also made for the CWP writing phase that followed in the few months following this last workshop.

Appendix B: Glossary

AOD	Analysis Object Data is a summary of the reconstructed event and contains sufficient information for common physics analyses.
ALPGEN	An event generator designed for the generation of Standard Model processes in hadronic collisions, with emphasis on final states with large jet multiplicities. It is based on the exact LO evaluation of partonic matrix elements, as well as top quark and gauge boson decays with helicity correlations.
BSM	Physics beyond the Standard Model (BSM) refers to the theoretical developments needed to explain the deficiencies of the Standard Model (SM), such as the origin of mass, the strong CP problem, neutrino oscillations, matter–antimatter asymmetry, and the nature of dark matter and dark energy.
Coin3D	A C++ object oriented retained mode 3D graphics API used to provide a higher layer of programming for OpenGL.
COOL	LHC Conditions Database Project, a subproject of the POOL persistency framework.
Concurrency Forum	Software engineering is moving towards a paradigm shift to accommodate new CPU architectures with many cores, in which concurrency will play a more fundamental role in programming languages and libraries. The forum on concurrent programming models and frameworks aims to share knowledge among interested parties that work together to develop 'demonstrators' and agree on technology so that they can share code and compare results.
CRSG	Computing Resources Scrutiny Group, a WLCG committee in charge of scrutinizing and assessing LHC experiment yearly resource requests to prepare funding agency decisions.
CSIRT	Computer Security Incident Response Team. A CSIRT provides a reliable and trusted single point of contact for reporting computer security incidents and taking the appropriate measures in response tothem.
CVMFS	The CERN Virtual Machine File System is a network file system based on HTTP and optimised to deliver experiment software in a fast, scalable, and reliable way through sophisticated caching strategies.
CWP	The Community White Paper (this document) is the result of an organised effort to describe the community strategy and a roadmap for software and computing R&D in HEP for the 2020s. This activity is organised under the umbrella of the HSF.
Deep Learning (DL)	one class of Machine Learning algorithms, based on a high number of neural network layers.
DNN	Deep Neural Network, class of neural networks with typically a large number of hidden layers through which data is processed.
DPHEP	The Data Preservation in HEP project is a collaboration for data preservation and long-term analysis.
EGI	European Grid Initiative. A European organisation in charge of delivering advanced computing services to support scientists, multinational projects and research infrastructures, partially funded by the European Union. It is operating both a grid infrastructure (many WLCG sites in Europe are also

	EGI sites) and a federated cloud infrastructure. It is also responsible for security incident response for these infrastructures (CSIRT).
FAIR	The Facility for Antiproton and Ion Research (FAIR) is located at GSI Darmstadt. It is an international accelerator facility for research with antiprotons and ions.
FAIR	An abbreviation for a set of desirable data properties: Findable, Accessible, Interoperable, and Re-usable.
FCC	Future Circular Collider, a proposed new accelerator complex for CERN, presently under study.
FCC-hh	A 100 TeV proton–proton collider version of the FCC (the “h” stands for “hadron”).
GAN	Generative Adversarial Networks are a class of artificial intelligence algorithms used in unsupervised machine learning, implemented by a system of two neural networks contesting with each other in a zero-sum game framework.
Geant4	A toolkit for the simulation of the passage of particles through matter.
GeantV	An R&D project that aims to fully exploit the parallelism, which is increasingly offered by the new generations of CPUs, in the field of detector simulation.
GPGPU	General-Purpose computing on Graphics Processing Units is the use of a Graphics Processing Unit (GPU), which typically handles computation only for computer graphics, to perform computation in applications traditionally handled by the Central Processing Unit (CPU). Programming for GPUs is typically more challenging, but can offer significant gains in arithmetic throughput.
HEPData	The Durham High Energy Physics Database is an open access repository for scattering data from experimental particle physics.
HERWIG	This is an event generator containing a wide range of Standard Model, Higgs and supersymmetric processes. It uses the parton-shower approach for initial- and final-state QCD radiation, including colour coherence effects and azimuthal correlations both within and between jets.
HL-LHC	The High Luminosity Large Hadron Collider is a proposed upgrade to the Large Hadron Collider to be made in 2026. The upgrade aims at increasing the luminosity of the machine by a factor of 10, up to 10^{35} cm^{-2}s^{-1}, providing a better chance to see rare processes and improving statistically marginal measurements.
HLT	High Level Trigger. The computing resources, generally a large farm, close to the detector which process the events in real-time and select those who must be stored for further analysis.
HPC	High-performance computing.
HS06	HEP-wide benchmark for measuring CPU performance based on the SPEC2006 benchmark (https://www.spec.org).
HSF	The HEP Software Foundation facilitates coordination and common efforts in High Energy Physics (HEP) software and computing internationally.
IML	The Inter-experimental LHC Machine Learning (IML) Working Group is focused on the development of modern state-of-the art machine learning methods, techniques and practices for high-energy physics problems.
IOV	Interval Of Validity, the period of time for which a specific piece of conditions data is valid.
JavaScript	A high-level, dynamic, weakly typed, prototype-based, multi-paradigm, and interpreted programming language. Alongside HTML and CSS, JavaScript is one of the three core technologies of World Wide Web content production.
Jupyter Notebook	This is a server–client application that allows editing and running notebook documents via a web browser. Notebooks are documents produced by the Jupyter Notebook App, which contain both computer code (e.g., python) and rich text elements (paragraph, equations, figures, links, etc...). Notebook documents are both human-readable documents containing the analysis description and the results (figures, tables, etc...) as well as executable documents which can be run to perform data analysis.
LHC	Large Hadron Collider, the main particle accelerator at CERN.
LHCONE	A set of network circuits, managed worldwide by the National Research and Education Networks, to provide dedicated transfer paths for LHC T1/T2/T3 sites on the standard academic and research physical network infrastructure.
LHCOPN	LHC Optical Private Network. It is the private physical and IP network that connects the Tier0 and the Tier1 sites of the WLCG.

MADEVENT	This is a multi-purpose tree-level event generator. It is powered by the matrix element event generator MADGRAPH, which generates the amplitudes for all relevant sub-processes and produces the mappings for the integration over the phase space.
Matplotlib	This is a Python 2D plotting library that provides publication quality figures in a variety of hardcopy formats and interactive environments across platforms.
ML	Machine learning is a field of computer science that gives computers the ability to learn without being explicitly programmed. It focuses on prediction making through the use of computers and emcompasses a lot of algorithm classes (boosted decision trees, neural networks...).
MONARC	A model of large-scale distributed computing based on many regional centers, with a focus on LHC experiments at CERN. As part of the MONARC project, a simulation framework was developed that provides a design and optimisation tool. The MONARC model has been the initial reference for building the WLCG infrastructure and to organise the data transfers around it.
OpenGL	Open Graphics Library is a cross-language, cross-platform Application Programming Interface (API) for rendering 2D and 3D vector graphics. The API is typically used to interact with a Graphics Processing Unit (GPU), to achieve hardware-accelerated rendering.
Openlab	CERN openlab is a public–private partnership that accelerates the development of cutting-edge solutions for the worldwide LHC community and wider scientific research.
P5	The Particle Physics Project Prioritization Panel is a scientific advisory panel tasked with recommending plans for U.S. investment in particle physics research over the next ten years.
PRNG	A PseudoRandom Number Generator is an algorithm for generating a sequence of numbers whose properties approximate the properties of sequences of random numbers.
PyROOT	A Python extension module that allows the user to interact with any ROOT class from the Python interpreter.
PYTHIA	A program for the generation of high-energy physics events, i.e., for the description of collisions at high energies between elementary particles such as e+, e-, p and pbar in various combinations. It contains theory and models for a number of physics aspects, including hard and soft interactions, parton distributions, initial- and final-state parton showers, multiparton interactions, fragmentation and decay.
QCD	Quantum Chromodynamics, the theory describing the strong interaction between quarks and gluons.
REST	Representational State Transfer web services are a way of providing interoperability between computer systems on the Internet. One of its main features is stateless interactions between clients and servers (every interaction is totally independent of the others), allowing for very efficient caching.
ROOT	A modular scientific software framework widely used in HEP data processing applications.
SAML	Security Assertion Markup Language. It is an open, XML-based, standard for exchanging authentication and authorisation data between parties, in particular, between an identity provider and a service provider.
SDN	Software-defined networking is an umbrella term encompassing several kinds of network technology aimed at making the network as agile and flexible as the virtualised server and storage infrastructure of the modern data center.
SHERPA	Sherpa is a Monte Carlo event generator for the Simulation of High-Energy Reactions of Particles in lepton–lepton, lepton–photon, photon–photon, lepton–hadron and hadron–hadron collisions.
SIMD	Single Instruction, Multiple Data (*SIMD*), describes computers with multiple processing elements that perform the same operation on multiple data points simultaneously.
SM	The Standard Model is the name given in the 1970s to a theory of fundamental particles and how they interact. It is the currently dominant theory explaining the elementary particles and their dynamics.
SWAN	Service for Web based ANalysis is a platform for interactive data mining in the CERN cloud using the Jupyter notebook interface.
TBB	Intel Threading Building Blocks is a widely used C++ template library for task parallelism. It lets you easily write parallel C++ programs that take full advantage of multicore performance.
TMVA	The Toolkit for Multivariate Data Analysis with ROOT is a standalone project that provides a ROOT-integrated machine learning environment for the processing and parallel evaluation of sophisticated multivariate classification techniques.

VecGeom	The vectorised geometry library for particle-detector simulation.
VO	Virtual Organisation. A group of users sharing a common interest (for example, each LHC experiment is a VO), centrally managed, and used in particular as the basis for authorisations in the WLCG infrastructure.
WebGL	The Web Graphics Library is a JavaScript API for rendering interactive 2D and 3D graphics within any compatible web browser without the use of plug-ins.
WLCG	The Worldwide LHC Computing Grid project is a global collaboration of more than 170 computing centres in 42 countries, linking up national and international grid infrastructures. The mission of the WLCG project is to provide global computing resources to store, distribute and analyse data generated by the Large Hadron Collider (LHC) at CERN.
X.509	A cryptographic standard which defines how to implement service security using electronic certificates, based on the use of a private and public key combination. It is widely used on web servers accessed using the https protocol and is the main authentication mechanism on the WLCG infrastructure.
x86_64	64-bit version of the x86 instruction set.
XRootD	Software framework that is a fully generic suite for fast, low latency and scalable data access.

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